

# Microsolvation of $\text{NO}_3^-$ :

## Structural exploration and bonding analysis

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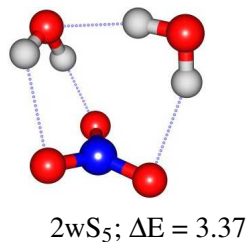
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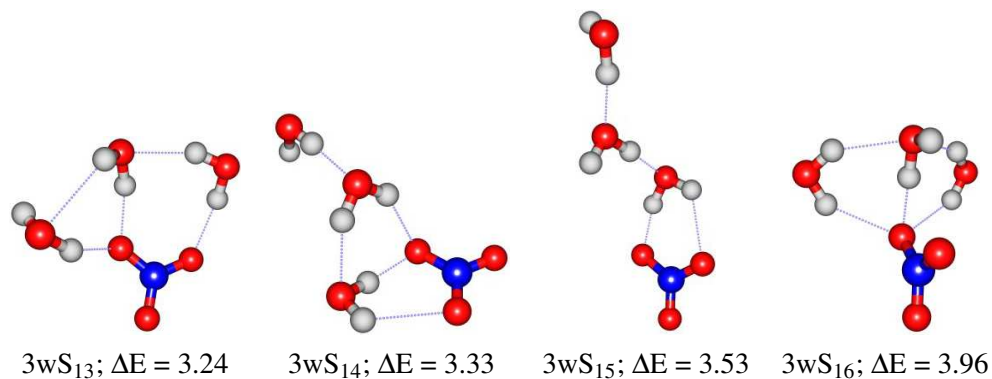
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<sup>§</sup> Universidad de Antioquia

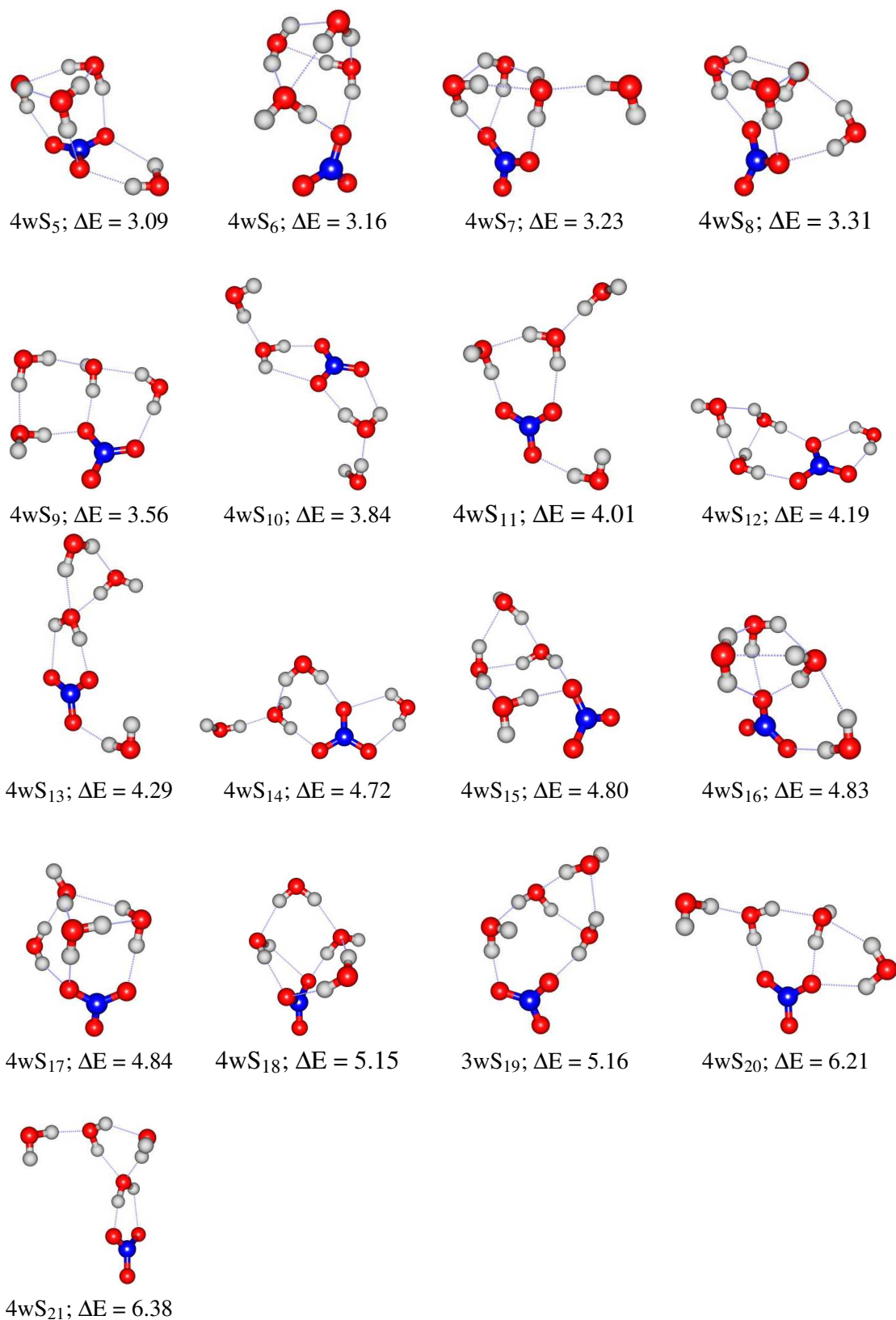
## Supporting Information



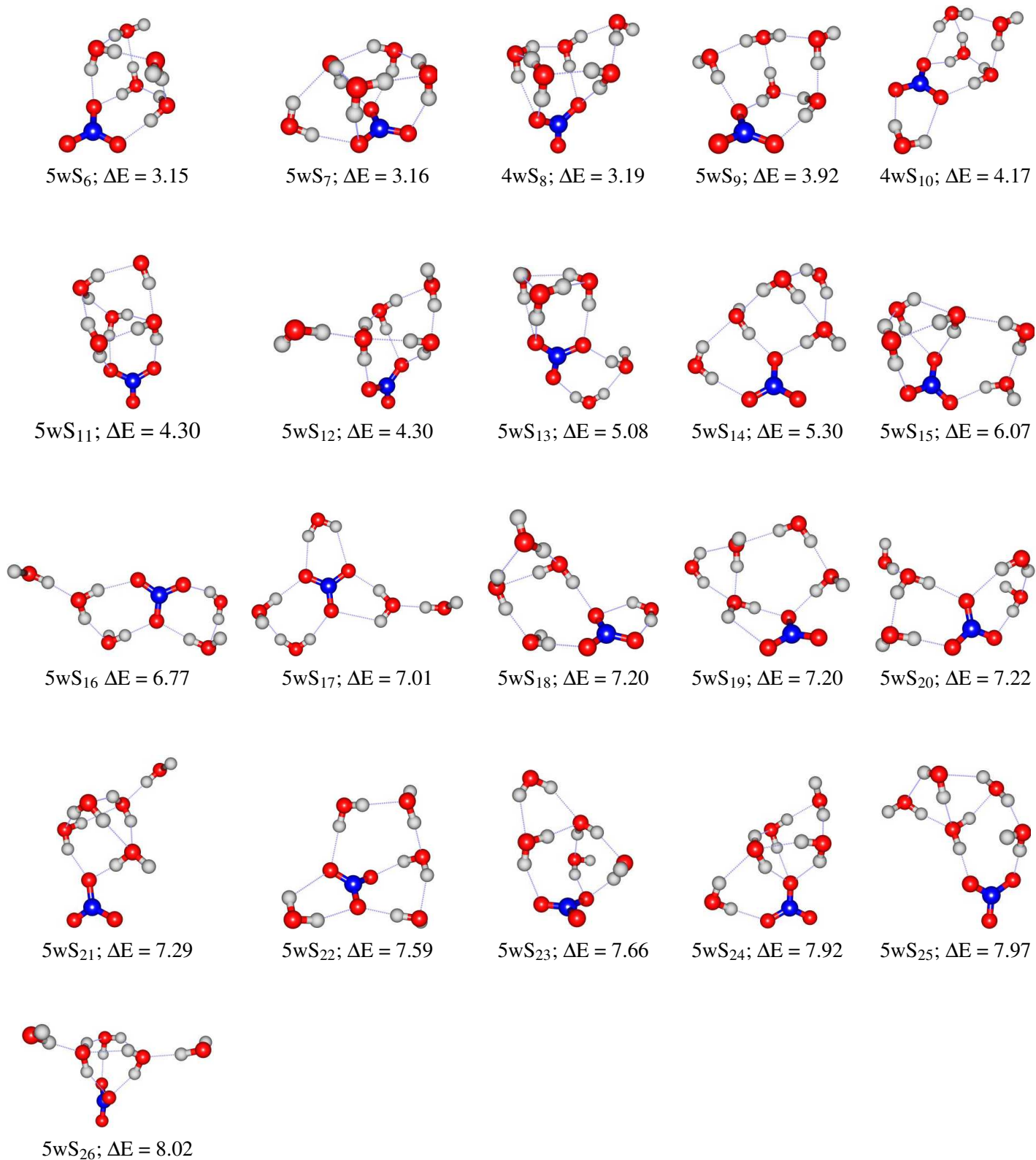
**Figure S1:** Structural motifs with energies larger than  $3 \text{ kcal mol}^{-1}$  of the global minimum on the potential energy surface for  $[\text{NO}_3(\text{H}_2\text{O})_2]^-$ . Dotted lines correspond to intermolecular contacts, those for which AIM predicts bonding paths. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries



**Figure S2:** Structural motifs with energies larger than  $3 \text{ kcal mol}^{-1}$  of the global minimum on the potential energy surface for  $[\text{NO}_3(\text{H}_2\text{O})_3]^-$ . Dotted lines correspond to intermolecular contacts, those for which AIM predicts bonding paths. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

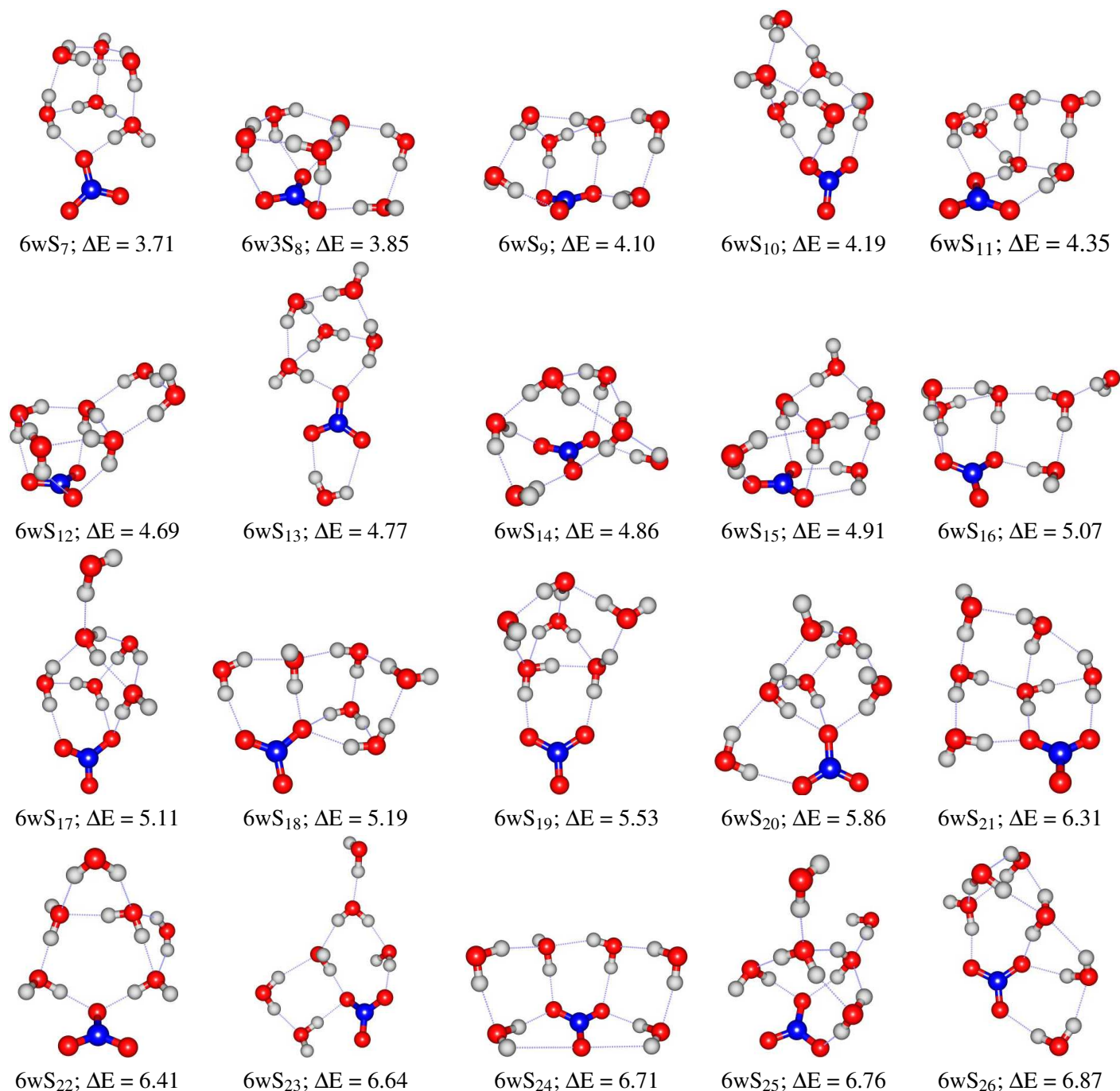


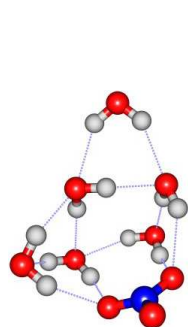
**Figure S3:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surface for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub>]<sup>-</sup>. Dotted lines correspond to intermolecular contacts, those for which AIM predicts bonding paths. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries



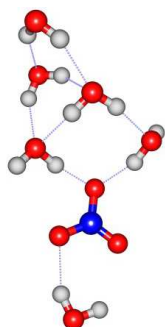
**Figure S4:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surface for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>5</sub>]<sup>-</sup>. Dotted lines correspond to intermolecular contacts, those for which AIM predicts bonding paths. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

**Figure S5:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surface for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>6</sub>]<sup>-</sup>. Dotted lines correspond to intermolecular contacts, those for which AIM predicts bonding paths. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

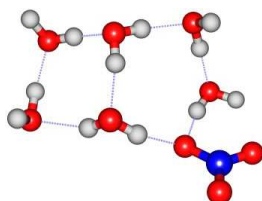




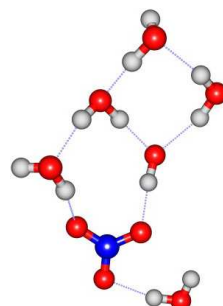
6wS<sub>27</sub>;  $\Delta E = 6.92$



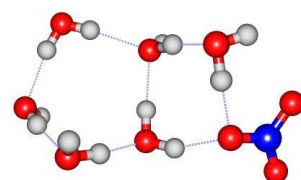
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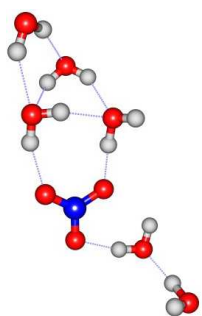
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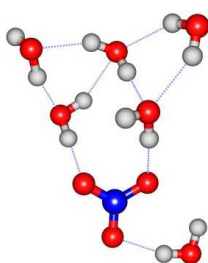
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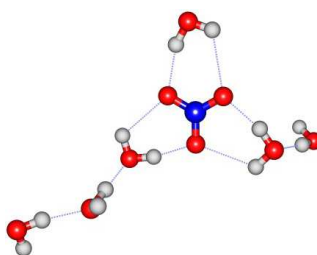
6wS<sub>31</sub>;  $\Delta E = 7.87$



6wS<sub>32</sub>;  $\Delta E = 8.13$



6wS<sub>33</sub>;  $\Delta E = 8.33$



6wS<sub>34</sub>;  $\Delta E = 8.53$

## Energetic Analysis

**Table S1:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surfaces for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>n</sub>]<sup>-</sup>. n=2,3,4. Isomer populations (%x<sub>i</sub>) estimated using standard Boltzmann distributions at 298 K, 1 atm. BE, BE<sub>H</sub>, BE<sub>G</sub>, refer to “binding energies” calculated as the difference between the energy of a particular cluster and the energy of its isolated moieties using the electronic energies, enthalpies of formation, and Gibbs energies, respectively. All energies in kcal mol<sup>-1</sup> and corrected for ZPEs. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

Structures	BE	ΔE	BE <sub>H</sub>	ΔE <sub>H</sub>	BE <sub>G</sub>	ΔE <sub>G</sub>	%x <sub>i</sub> E	%x <sub>i</sub> H	%x <sub>i</sub> G
2wS <sub>5</sub>	-24.67	3.37	-25.73	2.96	-7.76	4.31	0.29	0.50	0.06
3wS <sub>13</sub>	-35.91	3.24	-37.94	3.48	-9.71	5.08	0.17	0.20	0.01
3wS <sub>14</sub>	-35.83	3.33	-37.36	4.06	-11.15	3.64	0.14	0.08	0.16
3wS <sub>15</sub>	-35.63	3.53	-37.02	4.40	-12.10	2.69	0.10	0.04	0.80
3wS <sub>16</sub>	-35.20	3.96	-36.62	4.79	-10.20	4.50	0.05	0.02	0.04
4wS <sub>5</sub>	-48.25	3.09	-50.86	3.95	-13.82	2.12	0.45	0.11	1.45
4wS <sub>6</sub>	-48.35	3.16	-51.21	3.60	-12.77	3.17	0.39	0.20	0.24
4wS <sub>7</sub>	-48.28	3.23	-50.82	3.99	-13.61	2.33	0.34	0.10	0.99
4wS <sub>8</sub>	-48.20	3.31	-50.92	3.89	-12.31	3.63	0.30	0.12	0.11
4wS <sub>9</sub>	-47.95	3.56	-50.19	4.62	-13.45	2.49	0.19	0.03	0.76
4wS <sub>10</sub>	-47.66	3.84	-49.30	5.51	-15.94	0.00	0.12	0.00	49.72
4wS <sub>11</sub>	-47.50	4.01	-49.20	5.61	-15.52	0.42	0.09	0.00	25.54
4wS <sub>12</sub>	-47.32	4.19	-49.67	5.14	-13.02	2.92	0.06	0.01	0.38
4wS <sub>13</sub>	-47.22	4.29	-49.10	5.71	-14.18	1.77	0.06	0.00	2.59
4wS <sub>14</sub>	-46.79	4.72	-48.36	6.45	-14.36	1.58	0.02	0.00	3.57
4wS <sub>15</sub>	-46.71	4.80	-49.49	5.32	-11.23	4.71	0.02	0.01	0.02
4wS <sub>16</sub>	-46.68	4.83	-49.14	5.67	-12.10	3.84	0.02	0.00	0.08
4wS <sub>17</sub>	-46.67	4.84	-49.43	5.38	-11.10	4.84	0.02	0.01	0.01
4wS <sub>18</sub>	-46.36	5.15	-48.58	6.24	-11.44	4.51	0.01	0.00	0.03
4wS <sub>19</sub>	-46.35	5.16	-49.11	5.70	-11.11	4.83	0.01	0.00	0.01
4wS <sub>20</sub>	-46.30	5.21	-48.42	5.99	-12.47	3.47	0.01	0.00	0.15
4wS <sub>21</sub>	-45.12	6.38	-47.38	7.44	-12.26	3.68	0.00	0.00	0.10

**Table S2:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surfaces for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>5</sub>]<sup>-</sup>. Isomer populations (%*x<sub>i</sub>*) estimated using standard Boltzmann distributions at 298 K, 1 atm. BE, BE<sub>H</sub>, BE<sub>G</sub>, refer to “binding energies” calculated as the difference between the energy of a particular cluster and the energy of its isolated moieties using the electronic energies, enthalpies of formation, and Gibbs energies, respectively. All energies in kcal mol<sup>-1</sup> and corrected for ZPEs. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

Structures	BE	ΔE	BE <sub>H</sub>	ΔE <sub>H</sub>	BE <sub>G</sub>	ΔE <sub>G</sub>	% <i>x<sub>i</sub></i> E	% <i>x<sub>i</sub></i> H	% <i>x<sub>i</sub></i> G
5wS <sub>6</sub>	-60.53	3.15	-64.51	3.31	-16.05	0.96	0.48	0.38	7.09
5wS <sub>7</sub>	-60.52	3.16	-64.32	3.50	-13.27	3.75	0.48	0.28	0.07
5wS <sub>8</sub>	-60.49	3.19	-64.38	3.43	-17.02	0.00	0.45	0.31	35.30
5wS <sub>9</sub>	-59.76	3.92	-63.59	4.23	-13.17	3.85	0.13	0.08	0.06
5wS <sub>10</sub>	-59.51	4.17	-62.82	5.00	-13.65	3.36	0.09	0.02	0.13
5wS <sub>11</sub>	-59.38	4.30	-63.31	4.51	-15.28	1.73	0.07	0.05	1.96
5wS <sub>12</sub>	-59.38	4.30	-63.31	4.51	-13.60	3.42	0.07	0.05	0.12
5wS <sub>13</sub>	-58.61	5.08	-62.11	5.71	-14.88	2.13	0.02	0.01	1.03
5wS <sub>14</sub>	-58.38	5.30	-61.34	6.48	-13.63	3.39	0.01	0.00	0.12
5wS <sub>15</sub>	-57.61	6.07	-60.82	7.00	-11.97	5.05	0.00	0.00	0.01
5wS <sub>16</sub>	-56.91	6.77	-59.26	8.56	-11.75	5.27	0.00	0.00	0.01
5wS <sub>17</sub>	-56.67	7.01	-58.38	9.44	-11.65	5.36	0.00	0.00	0.00
5wS <sub>18</sub>	-56.48	7.20	-59.47	8.35	-14.10	2.91	0.00	0.00	0.27
5wS <sub>19</sub>	-56.48	7.20	-59.24	8.58	-15.71	1.31	0.00	0.00	3.98
5wS <sub>20</sub>	-56.46	7.22	-58.87	8.95	-15.31	1.70	0.00	0.00	2.09
5wS <sub>21</sub>	-56.39	7.29	-59.49	8.33	-14.87	2.15	0.00	0.00	0.97
5wS <sub>22</sub>	-56.09	7.59	-58.65	9.17	-14.54	2.48	0.00	0.00	0.58
5wS <sub>23</sub>	-56.03	7.66	-59.17	8.65	-15.66	1.35	0.00	0.00	3.73
5wS <sub>24</sub>	-55.76	7.92	-59.13	8.69	-15.13	1.89	0.00	0.00	1.52
5wS <sub>25</sub>	-55.71	7.97	-59.07	8.75	-14.40	2.61	0.00	0.00	0.45
5wS <sub>26</sub>	-55.66	8.02	-58.33	9.49	-15.52	1.50	0.00	0.00	2.89



**Table S3:** Structural motifs with energies larger than 3 kcal mol<sup>-1</sup> of the global minimum on the potential energy surfaces for [NO<sub>3</sub>(H<sub>2</sub>O)<sub>6</sub>]<sup>-</sup>. Isomer populations (%*x<sub>i</sub>*) estimated using standard Boltzmann distributions at 298 K, 1 atm. BE, BE<sub>H</sub>, BE<sub>G</sub>, refer to “binding energies” calculated as the difference between the energy of a particular cluster and the energy of its isolated moieties using the electronic energies, enthalpies of formation, and Gibbs energies, respectively. All energies in kcal mol<sup>-1</sup> and corrected for ZPEs. Data taken from the PBE0PBE1/Def2-PVTZ optimized geometries

Structures	BE	ΔE	BE <sub>H</sub>	ΔE <sub>H</sub>	BE <sub>G</sub>	ΔE <sub>G</sub>	% <i>x<sub>i</sub></i> E	% <i>x<sub>i</sub></i> H	% <i>x<sub>i</sub></i> G
6wS <sub>7</sub>	-69.81	3.71	-74.66	3.66	-14.61	3.75	0.09	0.10	0.09
6wS <sub>8</sub>	-69.68	3.85	-73.92	4.39	-15.34	3.02	0.07	0.03	0.31
6wS <sub>9</sub>	-69.42	4.10	-73.43	4.88	-15.18	3.17	0.05	0.01	0.24
6wS <sub>10</sub>	-69.33	4.19	-74.24	4.08	-14.18	4.18	0.04	0.05	0.05
6wS <sub>11</sub>	-69.18	4.35	-73.90	4.41	-14.49	3.86	0.03	0.03	0.08
6wS <sub>12</sub>	-68.83	4.69	-73.20	5.12	-14.66	3.70	0.02	0.01	0.10
6wS <sub>13</sub>	-68.76	4.77	-72.98	5.34	-14.23	4.12	0.02	0.01	0.05
6wS <sub>14</sub>	-68.67	4.86	-72.94	5.37	-14.01	4.34	0.01	0.01	0.03
6wS <sub>15</sub>	-68.61	4.91	-72.57	5.74	-15.69	2.67	0.01	0.00	0.56
6wS <sub>16</sub>	-68.45	5.07	-72.14	6.17	-16.35	2.01	0.01	0.00	1.66
6wS <sub>17</sub>	-68.42	5.11	-72.66	5.66	-15.00	3.36	0.01	0.00	0.18
6wS <sub>18</sub>	-68.33	5.19	-72.47	5.85	-15.57	2.79	0.01	0.00	0.46
6wS <sub>19</sub>	-68.00	5.53	-72.70	5.61	-13.96	4.40	0.00	0.00	0.03
6wS <sub>20</sub>	-67.66	5.86	-71.93	6.38	-14.15	4.21	0.00	0.00	0.04
6wS <sub>21</sub>	-67.21	6.31	-71.42	6.89	-13.59	4.77	0.00	0.00	0.02
6wS <sub>22</sub>	-67.11	6.41	-70.89	7.42	-14.38	3.97	0.00	0.00	0.06
6wS <sub>23</sub>	-66.88	6.64	-70.07	8.25	-15.90	2.45	0.00	0.00	0.82
6wS <sub>24</sub>	-66.82	6.71	-70.11	8.20	-14.66	3.70	0.00	0.00	0.10
6wS <sub>25</sub>	-66.77	6.76	-70.33	7.98	-15.16	3.20	0.00	0.00	0.23
6wS <sub>26</sub>	-66.66	6.87	-70.61	7.71	-13.26	5.10	0.00	0.00	0.01
6wS <sub>27</sub>	-66.61	6.92	-70.74	7.58	-12.68	5.68	0.00	0.00	0.00
6wS <sub>28</sub>	-66.52	7.01	-69.72	8.60	-15.46	2.90	0.00	0.00	0.38
6wS <sub>29</sub>	-66.04	7.49	-70.17	8.14	-13.50	4.86	0.00	0.00	0.01
6wS <sub>30</sub>	-65.85	7.67	-69.14	9.18	-14.84	3.52	0.00	0.00	0.14
6wS <sub>31</sub>	-65.66	7.87	-69.59	8.72	-14.06	4.30	0.00	0.00	0.04
6wS <sub>32</sub>	-65.40	8.13	-68.43	9.89	-15.67	2.69	0.00	0.00	0.56
6wS <sub>33</sub>	-65.19	8.33	-67.32	10.99	-18.36	0.00	0.00	0.00	49.80
6wS <sub>34</sub>	-64.99	8.53	-68.38	9.93	-13.65	4.71	0.00	0.00	0.02

**Table S4:** BSSE Correction for the lowest 6 energy isomer for the  $[\text{NO}_3(\text{H}_2\text{O})_6]^-$  at the PBE0PBE1/Def2-PVTZ level of theory.

Structures	BE	$\Delta E$	$\text{BE}_\text{H}$	$\Delta E_\text{H}$	$\text{BE}_\text{G}$	$\Delta E_\text{G}$
6wS <sub>1</sub>	-69.08	0.20	-73.95	0.16	-13.02	0.68
6wS <sub>2</sub>	-69.28	0.00	-74.11	0.00	-13.62	0.08
6wS <sub>3</sub>	-69.23	0.05	-74.05	0.06	-13.61	0.09
6wS <sub>4</sub>	-69.11	0.17	-73.82	0.29	-13.60	0.10
6wS <sub>5</sub>	-67.71	1.57	-72.62	1.49	-12.22	1.48
6wS <sub>6</sub>	-69.12	0.16	-74.03	0.08	-13.70	0.00

## Orbital Analysis

**Table S5:**  $n_O \rightarrow \sigma_{H-O}^*$  orbital interaction energies in the global minima and the lowest free energy

Donor ( $i$ ), $n_O$	Acceptor ( $j$ ), $\sigma_{H-O}^*$	$E_{ij}^{(2)}$ kcal/mol	Type
<b>5wS<sub>1</sub></b>			
O <sub>14</sub>	O <sub>11</sub> -H <sub>10</sub>	24.6	H <sub>2</sub> O...H-O-H
O <sub>2</sub>	O <sub>8</sub> -H <sub>9</sub>	13.8	H <sub>2</sub> O...H-O-H
O <sub>5</sub>	O <sub>14</sub> -H <sub>13</sub>	13.5	H <sub>2</sub> O...H-O-H
O <sub>8</sub>	O <sub>5</sub> -H <sub>4</sub>	13.2	H <sub>2</sub> O...H-O-H
O <sub>11</sub>	O <sub>2</sub> -H <sub>3</sub>	11.3	H <sub>2</sub> O...H-O-H
O <sub>17</sub>	O <sub>14</sub> -H <sub>15</sub>	5.67	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>18</sub>	O <sub>5</sub> -H <sub>6</sub>	5.19	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>17</sub>	O <sub>2</sub> -H <sub>1</sub>	4.12	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>17</sub>	O <sub>2</sub> -H <sub>1</sub>	2.81	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>17</sub>	O <sub>14</sub> -H <sub>15</sub>	2.80	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>17</sub>	O <sub>14</sub> -H <sub>15</sub>	2.07	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>17</sub>	O <sub>2</sub> -H <sub>1</sub>	1.65	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>19</sub>	O <sub>8</sub> -H <sub>7</sub>	0.66	NO <sub>3</sub> <sup>-</sup> ...H-O-H
<b>5wS<sub>16</sub></b>			
O <sub>17</sub>	O <sub>11</sub> -H <sub>13</sub>	12.20	H <sub>2</sub> O...H-O-H
O <sub>3</sub>	O <sub>17</sub> -H <sub>18</sub>	11.53	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>4</sub>	O <sub>8</sub> -H <sub>9</sub>	11.09	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>8</sub>	O <sub>5</sub> -H <sub>7</sub>	6.38	H <sub>2</sub> O...H-O-H
O <sub>4</sub>	O <sub>14</sub> -H <sub>16</sub>	3.68	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>4</sub>	O <sub>8</sub> -H <sub>9</sub>	3.19	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>2</sub>	O <sub>5</sub> -H <sub>6</sub>	1.87	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>4</sub>	O <sub>14</sub> -H <sub>16</sub>	1.29	NO <sub>3</sub> <sup>-</sup> ...H-O-H

**Table S6:**  $n_O \rightarrow \sigma_{H-O}^*$  orbital interaction energies in the global minima and the lowest free energy structures for the interactions between nitrate ion and 6 water molecules.

Donor ( $i$ ), $n_O$	Acceptor ( $j$ ), $\sigma_{H-O}^*$	$E_{ij}^{(2)}$ kcal/mol	Type
<b>6wS<sub>1</sub></b>			
O <sub>13</sub>	O <sub>7</sub> -H <sub>9</sub>	14.8	H <sub>2</sub> O...H-O-H
O <sub>18</sub>	O <sub>3</sub> -H <sub>1</sub>	14.7	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>18</sub>	O <sub>7</sub> -H <sub>8</sub>	14.7	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>4</sub>	O <sub>13</sub> -H <sub>14</sub>	13.2	H <sub>2</sub> O...H-O-H
O <sub>17</sub>	O <sub>20</sub> -H <sub>21</sub>	5.19	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>19</sub>	O <sub>4</sub> -H <sub>6</sub>	4.12	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>7</sub>	O <sub>10</sub> -H <sub>12</sub>	2.76	H <sub>2</sub> O...H-O-H
O <sub>1</sub>	O <sub>10</sub> -H <sub>11</sub>	2.30	H <sub>2</sub> O...H-O-H
O <sub>20</sub>	O <sub>4</sub> -H <sub>5</sub>	2.07	H <sub>2</sub> O...H-O-H
O <sub>19</sub>	O <sub>4</sub> -H <sub>6</sub>	1.65	NO <sub>3</sub> <sup>-</sup> ...H-O-H
<b>6wS<sub>33</sub></b>			
O <sub>20</sub>	O <sub>11</sub> -H <sub>13</sub>	21.1	H <sub>2</sub> O...H-O-H
O <sub>5</sub>	O <sub>2</sub> -H <sub>16</sub>	15.1	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>8</sub>	O <sub>1</sub> -H <sub>3</sub>	13.4	H <sub>2</sub> O...H-O-H
O <sub>14</sub>	O <sub>17</sub> -H <sub>19</sub>	12.0	H <sub>2</sub> O...H-O-H
O <sub>6</sub>	O <sub>8</sub> -H <sub>9</sub>	11.7	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>7</sub>	O <sub>11</sub> -H <sub>13</sub>	6.30	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>6</sub>	O <sub>8</sub> -H <sub>9</sub>	2.25	NO <sub>3</sub> <sup>-</sup> ...H-O-H
O <sub>7</sub>	O <sub>11</sub> -H <sub>13</sub>	1.13	NO <sub>3</sub> <sup>-</sup> ...H-O-H

Microsolvation of NO<sub>3</sub><sup>-</sup>:  
Structural exploration and bonding analysis

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Corresponding author: e-mail: albeiro.restrepo@udea.edu.co,

Cartesian coordinates for all clusters

Level of theory:

PBE0PBE/DEF2TZVP

[NO<sub>3</sub>(H<sub>2</sub>O)<sub>1</sub>]- Clusters

W1\_S1

-1 1

N	0.77389300	0.00274600	0.00002000
O	0.11557600	-1.06399700	0.00015500
O	2.00876000	-0.03585000	-0.00018600
O	0.17746800	1.09962100	0.00014400
O	-2.51110000	-0.01818100	-0.00011100
H	-1.97010300	0.78254600	-0.00008700
H	-1.77277100	-0.65451000	-0.00007300

W1\_S2

N	0.79941400	0.00774000	-0.00046400
O	0.03964600	-0.99450700	-0.00212000
O	0.30504000	1.14923900	-0.00195300
O	2.02426400	-0.15294800	0.00279300
O	-2.56347500	-0.06846700	0.00156900
H	-2.40462900	0.87841400	0.00450800
H	-1.63506500	-0.39913200	-0.00357100

S1\_S3

N	0.87553000	0.00586000	-0.01394400
O	0.76670300	1.23910600	-0.00236600
O	-0.15462900	-0.70897000	-0.13614200
O	1.98117500	-0.54031000	0.09125700
O	-2.76672600	0.09004100	0.01033000
H	-2.95042900	-0.71205600	0.50222100
H	-1.79045800	0.03210000	-0.10924900

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[NO<sub>3</sub>(H<sub>2</sub>O)<sub>2</sub>]- Clusters

W2\_S1

-1 1

O	-2.91892900	-0.98649100	0.00002800
H	-2.51119200	-0.10187700	0.00002000
H	-2.11220500	-1.51258900	0.00000000
N	0.00731100	0.62117800	-0.00001600
O	-1.09427700	1.19909000	-0.00000100
O	0.04980900	-0.63176600	-0.00005500

O	1.05543900	1.28023300	0.00002000
O	2.88373800	-1.04068900	0.00001600
H	1.92819400	-1.21952500	-0.00001800
H	2.83777700	-0.07726200	0.00003900

W2\_S2

-1 1			
N	1.23173400	-0.03666600	0.01569500
O	2.42938800	-0.29492500	-0.07486900
O	0.76114500	0.97399900	-0.56167600
O	0.46993200	-0.76884400	0.68560800
O	-1.79817800	1.45391300	0.25524300
H	-1.75943900	0.97984500	1.09001400
H	-0.88344500	1.31583000	-0.09331300
O	-2.16219000	-1.39089400	-0.37885300
H	-1.24128400	-1.38322300	-0.07004400
H	-2.33874800	-0.44178800	-0.44014300

W2\_S3

-1 1			
O	1.43673300	0.17186900	0.44728500
H	0.69482700	-0.46813300	0.33499200
H	0.92860200	0.97963100	0.29637900
O	4.02643800	-0.09496800	-0.37496800
H	3.06051700	-0.00281100	-0.21570800
H	4.37069400	-0.24756200	0.50639000
N	-1.71025900	-0.02411400	-0.04974800
O	-0.96564700	-1.02791900	0.09730600
O	-1.21019100	1.11874000	-0.04458500
O	-2.92268700	-0.17926200	-0.19676400

W2\_S4

-1 1			
N	0.23158900	-0.90014000	-0.01968400
O	-0.53322600	-1.86268500	-0.00380200
O	-0.23734500	0.26560600	-0.17238100
O	1.45638300	-1.04592100	0.10939700
O	2.14770300	1.82009100	0.00376100
H	1.21536200	1.56479100	-0.10644200
H	2.51251600	0.93374300	0.11156200
O	-2.91438500	1.01049900	0.02703800
H	-2.07252200	0.53173000	-0.11761600
H	-2.62952100	1.76999900	0.53817000

W2\_S5

-1 1			
O	1.85263500	1.51245500	-0.10054400
H	1.92295000	0.54612900	-0.05914400
H	0.90357100	1.67078000	-0.01458900
O	1.58320000	-1.47413300	-0.01624200
H	1.06111600	-1.50748100	-0.82683900
H	0.86516400	-1.30916500	0.62871600
N	-1.04813200	0.01163100	0.03453100
O	-1.28047400	1.22813900	-0.02411000
O	-0.72582300	-0.50706100	1.13055300
O	-1.10652200	-0.69461100	-0.98589000

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[NO3(H2O)\_3]- Clusters

W3\_S1

-1 1

H	-2.16917600	-1.09907900	-0.39244100
O	-1.83711900	-1.02443700	-1.30046600
H	-0.87802800	-1.03986500	-1.13872800
H	-1.81134300	0.39608200	1.19847700
O	-1.74656200	-0.50217400	1.57019200
H	-0.84212300	-0.74764400	1.31491300
H	-0.53410500	1.57448800	-0.17335400
O	-1.50497800	1.70045200	-0.23210700
H	-1.76795900	1.00429500	-0.85270200
N	1.58346500	-0.04565800	-0.00832100
O	1.23027300	1.14884000	-0.08927600
O	2.77028400	-0.34573900	0.02827900
O	0.70291200	-0.94802600	0.03613700

W3\_S2

O	-1.21897500	0.24688200	0.00376300
O	0.82472800	0.93285200	-0.00343600
N	0.00097600	-0.00011200	0.00169700
O	0.39691700	-1.18001100	0.00480600
O	-0.87407400	3.25667900	-0.00081600
H	-0.12190200	2.64125600	-0.00286700
H	-1.59566800	2.62021900	0.00197700
O	-2.38803900	-2.38224500	-0.00386400
H	-2.22057000	-1.42471900	-0.00058300
H	-1.47998200	-2.70002300	-0.00264200
O	3.25822200	-0.87349200	-0.00111400
H	2.34713000	-1.21205200	0.00154500
H	3.07392100	0.07077700	-0.00403700

W3\_S3

-1 1

H	2.92407100	0.33177200	0.68805700
O	3.08280500	-0.60603300	0.86730400
H	2.28219900	-1.00395600	0.49547300
H	-3.01592100	-0.03435800	0.22876200
O	-3.48024100	0.78573700	0.47018100
H	-2.72564500	1.37925400	0.53232900
H	1.09085200	1.38175300	-0.22594800
O	1.97138600	1.75236800	-0.46306800
H	2.23439500	1.19619100	-1.20065500
N	-0.49629700	-0.61032500	-0.24242500
O	-0.47844500	0.60470400	0.07331300
O	0.55690400	-1.17838200	-0.56872500
O	-1.56689300	-1.23069300	-0.23163500

W3\_S4

H	-0.50206700	1.72025300	-0.33204200
O	-1.46880000	1.63173500	-0.39739500
H	-1.58199600	0.82482400	-0.92851500
H	-1.58387700	-1.21463900	-0.25032200
O	-1.47051100	-1.15902600	-1.21475900
H	-0.50386700	-1.14856600	-1.32429700

H	-0.50563200	-0.57345900	1.65723400
O	-1.47201900	-0.47164100	1.61010000
H	-1.58316700	0.39237900	1.17745600
N	1.34571300	-0.00035600	0.00053800
O	1.33835300	1.24308900	0.06597000
O	1.34012400	-0.56528300	-1.10892700
O	1.33793000	-0.67866100	1.04460000

W3\_S5  
-1 1

H	-3.33465900	0.56272500	-0.01265000
O	-3.91224200	1.04799200	-0.64003600
H	-3.31102600	1.29157100	-1.34609600
H	-1.92571000	-1.18176900	0.60093600
O	-2.12025600	-0.31524000	0.97710600
H	-1.22883100	0.08797500	0.88332200
H	2.97790800	0.82551600	-0.20815100
O	3.13552700	1.74181900	0.08053700
H	2.26549600	1.94037200	0.44009600
N	0.89537700	-0.75997100	-0.12222100
O	0.49168300	0.30857400	0.40577400
O	0.12675700	-1.72277500	-0.23412400
O	2.06467800	-0.83619400	-0.52699500

W3\_S6

H	0.40564500	1.32294400	-0.48289900
O	1.03333400	1.79897900	0.09725000
H	0.75494500	1.47211600	0.95903000
H	2.71814300	0.75077100	-0.03360800
O	3.32994600	-0.00149100	0.00065700
H	2.71560700	-0.75188700	0.03182500
H	0.74975900	-1.46810900	-0.95822200
O	1.03191400	-1.79816200	-0.09880400
H	0.40620000	-1.32461900	0.48523700
N	-1.65742800	0.00010600	0.00026800
O	-1.01726900	-0.25596200	1.05109700
O	-2.88082400	-0.00039200	-0.00088100
O	-1.01563900	0.25678400	-1.04972400

W3\_S7

H	-0.43438800	-2.43358000	-0.17949200
O	-0.96606100	-1.94757100	0.45604900
H	-0.38073100	-1.17574100	0.63884000
H	-2.45176900	-0.92802100	-0.26740100
O	-3.07904400	-0.25272000	-0.57678200
H	-2.55689200	0.56242200	-0.55444700
H	-1.75240300	2.03340000	0.99068400
O	-1.35949500	2.08261400	0.11656400
H	-0.52792200	1.56931000	0.21405000
N	1.67532900	0.04208900	-0.03902100
O	2.40525100	0.98085500	-0.33688800
O	1.92700800	-1.11986600	-0.37012500
O	0.61944100	0.26638800	0.64004700

W3\_S8

H	-2.10481100	-0.97130400	0.22197000
O	-2.62850100	-0.41335700	0.84252700



H	-2.00620500	-0.21817200	1.54735800
H	-0.69875400	1.77124900	-0.45598100
O	-1.56971300	2.14795000	-0.26060600
H	-2.09455200	1.37653800	-0.00293800
H	-0.28942200	-2.19555600	-0.23991300
O	-0.91895000	-1.76313200	-0.83008600
H	-0.39484700	-0.94507500	-1.01200200
N	1.57823500	0.04695100	0.07313800
O	2.44213900	0.84582000	0.41391000
O	1.52035500	-1.09453200	0.56299500
O	0.72228800	0.38395900	-0.80004800

W3\_S9

H	2.15476300	-0.67074900	-0.43428900
O	2.71120800	0.07543000	-0.69498800
H	2.21898800	0.83941700	-0.35523900
H	-1.82544800	1.11567100	-1.36585000
O	-1.83070100	1.66886900	-0.57924400
H	-1.69009900	0.99245500	0.11772800
H	0.54434100	1.18177200	1.03902300
O	0.87384600	1.96770700	0.57183600
H	0.11762100	2.17147100	0.00042500
N	-0.49918000	-1.15138600	0.20357300
O	0.55020900	-1.79329300	0.31888400
O	-1.26835900	-1.33590000	-0.74388100
O	-0.78944100	-0.27910500	1.07404100

W3\_S10

H	1.18882400	0.04779300	0.88231500
O	2.07505900	0.44755600	0.79687600
H	1.87661200	1.22815000	0.25532100
H	2.38555000	-1.21075000	-0.28043200
O	2.11589000	-2.05426400	-0.67807200
H	1.16729600	-2.05189700	-0.50390800
H	-0.10215700	1.87358000	-0.46956000
O	0.61917000	2.54816900	-0.50251000
H	0.43577200	3.10181800	0.25912100
N	-1.47277100	-0.34615000	0.09279800
O	-2.48815000	-1.02376200	-0.01030900
O	-1.48814900	0.86423800	-0.23688900
O	-0.41413400	-0.85264200	0.53184900

W3\_S11

-1 1			
H	-2.81514200	-0.77984300	0.61326200
O	-3.28078900	-0.03828900	1.02948100
H	-2.75799500	0.70859400	0.70948800
H	-1.18626500	2.17124300	-1.16674400
O	-1.26733300	1.43117400	-0.56393400
H	-0.32933600	1.21688300	-0.29758100
H	-0.56850000	-1.41466600	-0.47941800
O	-1.47869100	-1.41704800	-0.82987800
H	-1.58566400	-0.48844200	-1.08067200
N	1.86121000	-0.04720200	0.15030000
O	3.06859800	-0.07445300	0.36552400
O	1.28337000	1.06359200	0.00004200
O	1.20164900	-1.10039600	0.07996000

## W3\_S12

-1 1

H	0.23968700	-1.54983200	-0.11991200
O	0.97889500	-1.79597500	0.47733500
H	0.83461900	-1.17591600	1.19844700
H	2.64766000	-0.91587800	-0.10961500
O	3.31124900	-0.22306200	-0.25861800
H	2.76012900	0.57171000	-0.33137700
H	0.51692700	1.36693900	-0.00743200
O	1.31819100	1.90737800	-0.18963000
H	1.41781800	2.43003700	0.60817600
N	-1.73193800	0.00560800	-0.05198400
O	-1.29888300	-0.88164700	-0.81604000
O	-0.92190100	0.61242000	0.70109200
O	-2.92421000	0.28509700	-0.02343900

## W3\_S13

-1 1

H	0.44543600	1.20020500	0.63414500
O	0.73038600	2.12069200	0.45350700
H	1.38638800	1.98187000	-0.23784300
H	-1.17824300	2.32956500	-0.21562600
O	-2.07531800	2.04475000	-0.44022000
H	-2.04087700	1.09073500	-0.27009600
H	2.07062600	-0.37935400	-0.30669800
O	2.90606600	0.09056200	-0.50232100
H	3.18654800	0.38647900	0.36649500
N	-0.53889700	-1.32397600	0.11888100
O	-1.67923300	-0.84335900	0.10492500
O	-0.32334500	-2.48269700	-0.21795400
O	0.42924400	-0.59765700	0.50174500

## W3\_S14

-1 1

H	-0.46510600	2.36334800	0.23856600
O	0.26130600	2.06444900	-0.31720500
H	-0.11437800	1.20709300	-0.62942000
H	1.41644600	0.84667500	0.66008900
O	1.68385400	-0.05692000	0.90778600
H	0.94948100	-0.57202700	0.53884400
H	3.30053100	-0.50918900	0.24704500
O	4.13166000	-0.72579600	-0.22519500
H	3.88610500	-0.64179400	-1.14807500
N	-1.87388900	-0.42168900	-0.08321100
O	-0.73239800	-0.45809100	-0.64017200
O	-2.31323600	0.66869700	0.31022000
O	-2.51316800	-1.46012400	0.04899500

## W3\_S15

-1 1

H	0.03361200	1.21768200	0.57759500
O	0.40655100	0.47809600	1.07421300
H	-0.37177800	-0.13654400	1.00049000
H	1.72412800	-0.18259500	0.30855100
O	2.46694800	-0.61517400	-0.19482200
H	2.04329600	-0.99488600	-0.96618000

H	4.12869800	0.02417900	-0.39081000
O	5.08478000	0.23555700	-0.40508300
H	5.41569000	-0.19754000	0.38329400
N	-2.48159400	-0.01215000	-0.15848200
O	-3.58895000	-0.30843000	-0.60113400
O	-1.84864000	-0.84493300	0.54769500
O	-1.97100000	1.09922800	-0.39631500

W3\_S16  
-1 1

H	0.66380100	1.93848300	-0.92797300
O	1.40506700	2.47094800	-0.61344400
H	1.77341900	1.90116000	0.07525500
H	0.90636600	0.02157300	0.43262600
O	1.66314000	0.04082800	1.07589600
H	1.18769000	0.02080400	1.91102500
H	0.80463900	-1.91075100	-0.94786900
O	1.58032300	-2.38554400	-0.62491700
H	1.89846000	-1.78895500	0.06654200
N	-1.45445100	-0.03896400	0.03141400
O	-1.36257000	-0.05099100	1.26368200
O	-2.53544800	-0.05367200	-0.54272100
O	-0.38216400	-0.01026600	-0.66218400

[NO3(H2O)\_4]- Clusters

W4\_S1  
-1 1

O	1.67568600	1.11187000	0.12260300
O	0.95941300	-0.17442700	-1.45146300
N	1.45644100	-0.03013500	-0.31214900
O	1.71034000	-1.03005000	0.37882500
O	-1.55637900	1.30860400	-1.22858500
H	-0.64547400	1.11542800	-1.50243200
H	-1.45354900	1.52549100	-0.28047100
O	-0.83833600	1.56499900	1.49814500
H	0.08969900	1.61748800	1.21922400
H	-0.94047600	0.62041300	1.73235500
O	-0.82890600	-1.25470500	1.75339000
H	0.11866300	-1.30857100	1.55074000
H	-1.23534300	-1.45762300	0.88686500
O	-1.57801600	-1.50727900	-0.96088000
H	-1.83502000	-0.57393100	-1.09546300
H	-0.64399900	-1.47984400	-1.22206700

W4\_S2  
-1 1

O	1.46351900	-1.75111900	1.05704500
H	0.50035400	-1.69123600	0.96323000
H	1.73845800	-1.62188500	0.12971300
O	1.46167000	1.75146100	-1.05777000
H	1.73871200	1.62335500	-0.13098100
H	0.49873400	1.69029500	-0.96188200
N	-1.75386000	-0.00023600	0.00010700
O	-2.97548000	-0.00018400	0.00068500
O	-1.11701600	1.07039700	0.16630500
O	-1.11717300	-1.07086600	-0.16643500

O	1.37689600	1.02076500	1.67276400
H	0.45233400	1.06445700	1.37565200
H	1.57337000	0.06709300	1.60733200
O	1.37647600	-1.02036700	-1.67262200
H	0.45185400	-1.06466900	-1.37574800
H	1.57207200	-0.06645100	-1.60784300

W4\_S3

-1 1			
H	-0.89067100	-0.34976300	1.56396200
O	-1.86174500	-0.26342400	1.54583900
H	-2.10725200	-0.80446400	0.77766700
H	-1.80645800	-0.20249600	-1.27193200
O	-1.91711100	-1.16817500	-1.21165500
H	-1.02499500	-1.50044900	-1.02481000
H	1.10790100	1.60282300	0.54363700
O	1.09266700	2.33785000	-0.10380400
H	1.65359200	1.96679600	-0.79289800
H	-0.76120100	1.98298100	-0.54206100
O	-1.67103800	1.64156500	-0.60222700
H	-1.82209500	1.22216000	0.26370400
N	1.31331000	-0.79081000	0.10110900
O	0.95646700	-0.13482200	1.12040000
O	0.72349400	-1.84380600	-0.17696300
O	2.23451800	-0.36692800	-0.59971900

W4\_S4

-1 1			
N	-0.89025700	-0.63140400	0.01228100
O	-1.94215600	-1.27433100	0.05198100
O	0.20688100	-1.23073300	0.01097700
O	-0.91581200	0.61654800	-0.02682000
O	2.67588100	-0.49528400	-1.36570700
H	3.01854900	-0.51903700	-0.45798300
H	1.77135700	-0.81664500	-1.22736500
O	2.53554000	-0.16195700	1.51785600
H	1.73123200	-0.66165500	1.31366400
H	2.30140800	0.72645000	1.19133200
O	1.58079000	1.93884300	-0.14775000
H	2.01575400	1.38373000	-0.81294000
H	0.68520100	1.55060100	-0.09663400
O	-3.96489500	0.78222600	-0.03345600
H	-3.23307600	1.40583700	-0.05715500
H	-3.46845000	-0.05194500	0.00446100

W4\_S5

-1 1			
O	-2.79844500	0.49417100	-0.24433400
H	-2.09560000	1.16271900	-0.21521100
H	-2.42563800	-0.18158600	-0.83774100
N	0.56657500	0.94909000	-0.00896000
O	0.95713200	0.51645600	1.09313300
O	1.00464500	0.44056400	-1.06505300
O	-0.26187900	1.86573100	-0.06148300
O	-1.34530000	-1.21861700	1.57166100
H	-1.99962600	-0.59493000	1.21100000
H	-0.54167900	-0.68158800	1.65637800

O	3.40935000	-0.81527000	-0.02148400
H	2.73791700	-0.49749100	-0.64442300
H	2.96408100	-0.60365500	0.80589000
O	-1.11351300	-1.59013700	-1.28997000
H	-0.33821500	-1.02720600	-1.44020700
H	-1.08317800	-1.76308500	-0.33272400

W4\_S6

-1 1			
H	-0.05670100	-0.88410900	-0.31082300
O	0.61706900	-1.61923300	-0.21847600
H	0.06765800	-2.40266100	-0.14932500
H	0.33111800	1.64868200	0.01646000
O	1.25163200	1.91857300	0.17831000
H	1.54774000	1.32832000	0.88952900
H	2.29354200	0.81095800	-1.04423300
O	2.79767900	0.02740400	-1.33257400
H	2.14154400	-0.68233900	-1.27992700
H	1.74932600	-0.95189400	1.19883800
O	2.46909400	-0.39117500	1.53937000
H	3.00235500	-0.27555500	0.73831400
N	-2.22144100	0.06097900	-0.03661100
O	-1.04643600	0.40307700	-0.39386000
O	-3.06401700	0.92706700	0.15745200
O	-2.46583200	-1.14299500	0.09445900

W4\_S7

-1 1			
O	-2.36977900	-1.50833200	-0.37898600
H	-2.52144800	-0.66296200	-0.82168500
H	-1.42049900	-1.64205700	-0.53918800
N	1.29483200	-0.89441300	-0.01432800
O	1.20980500	-0.01281800	0.87464900
O	2.23950900	-1.66417600	-0.04475900
O	0.38185300	-0.97048100	-0.88100600
O	-1.35948200	1.28968600	-0.98288100
H	-0.67091600	0.60353500	-1.07599800
H	-1.53225200	1.26500500	-0.02432300
O	-1.49744500	0.37078700	1.71515400
H	-1.89894400	-0.40442300	1.29357600
H	-0.54187000	0.24578900	1.56471400
O	1.13248200	2.78481700	-0.27886700
H	1.35780500	1.96324100	0.17796400
H	0.26874600	2.57689400	-0.66119400

W4\_S8

-1 1			
O	-2.36977900	-1.50833200	-0.37898600
H	-2.52144800	-0.66296200	-0.82168500
H	-1.42049900	-1.64205700	-0.53918800
N	1.29483200	-0.89441300	-0.01432800
O	1.20980500	-0.01281800	0.87464900
O	2.23950900	-1.66417600	-0.04475900
O	0.38185300	-0.97048100	-0.88100600
O	-1.35948200	1.28968600	-0.98288100
H	-0.67091600	0.60353500	-1.07599800
H	-1.53225200	1.26500500	-0.02432300

O	-1.49744500	0.37078700	1.71515400
H	-1.89894400	-0.40442300	1.29357600
H	-0.54187000	0.24578900	1.56471400
O	1.13248200	2.78481700	-0.27886700
H	1.35780500	1.96324100	0.17796400
H	0.26874600	2.57689400	-0.66119400

W4\_S9

-1	1		
H	2.93179000	0.70091900	-0.25693100
O	2.93635000	1.63729200	-0.51513200
H	2.00408700	1.89020700	-0.47268200
H	1.60889100	-0.98908500	0.55769400
O	2.55686500	-1.12532500	0.33766100
H	2.51180500	-1.79243500	-0.35108400
H	-0.09956700	1.14975000	0.29603100
O	0.03294500	2.11685100	0.14828400
H	0.18167700	2.46812700	1.02906400
H	-2.72906700	0.80314000	-0.06398600
O	-2.91874200	1.75383300	-0.04992600
H	-2.03579800	2.13990600	-0.11548500
N	-0.82507800	-1.35006500	-0.01150900
O	-0.34260500	-2.43031600	-0.33662300
O	-0.10522800	-0.52710500	0.64139400
O	-1.98436900	-1.04023900	-0.29341500

W4\_S10

-1	1		
O	-4.60856200	1.35935600	-0.48881000
H	-4.13475100	1.30140500	-1.32027600
H	-3.98129000	0.96973400	0.15572200
O	4.76486700	0.91583200	0.74390800
H	4.47038300	0.26004500	1.37827500
H	4.02003300	0.96426900	0.10872500
N	0.00691700	-1.02801200	-0.15445000
O	1.07527500	-1.39688700	-0.67526200
O	-0.16094100	0.19066300	0.10409400
O	-0.87728400	-1.84695300	0.10549500
O	-2.71053800	0.18375100	1.16683400
H	-1.80650300	0.38968000	0.84649100
H	-2.70497900	-0.77113400	1.03596200
O	2.53518700	0.92285200	-0.91591400
H	2.13068600	0.02727900	-0.92240900
H	1.81396800	1.42589900	-0.52410500

W4\_S11

-1	1		
N	-1.45061100	0.53750600	-0.28499000
O	-2.64417700	0.31319300	-0.51326200
O	-0.98344600	1.67201000	-0.51261700
O	-0.71877900	-0.36311800	0.17353100
O	2.11856500	-0.20199500	0.36369800
H	2.15366800	0.76938300	0.37036000
H	1.16776900	-0.36997300	0.23687000
O	4.18009900	-1.79696800	-0.53250100
H	4.21699000	-2.34505400	0.25288300
H	3.43761600	-1.18726000	-0.33983600

O	-3.02854600	-2.35737900	0.46918900
H	-2.08476000	-2.38208000	0.65120600
H	-3.10031800	-1.46619000	0.08636100
O	1.40292500	2.53135800	0.46215800
H	0.56105300	2.20424600	0.06423500
H	1.18913100	2.63758200	1.39128900

W4\_S12

-1 1			
H	-0.69173500	1.31601600	-0.49526000
O	-1.54666800	1.74103400	-0.70052700
H	-2.07787300	1.61649200	0.09831100
H	-2.12018300	-0.11374700	-1.16115100
O	-2.30167800	-0.99866900	-0.80316400
H	-1.40797500	-1.29028600	-0.51767300
H	-4.34332700	0.62225900	0.79726700
O	-3.48736700	0.44441800	1.19167200
H	-3.08758300	-0.23201100	0.59603400
H	3.46206600	0.42487200	0.28525300
O	3.78167600	1.33955300	0.19432300
H	2.95529900	1.77929700	-0.02533600
N	1.15320500	-0.78645300	0.04449600
O	0.25851100	-1.64912700	0.00042000
O	2.31272400	-1.11784400	0.31942300
O	0.88766200	0.41342100	-0.18826200

W4\_S13

-1 1			
H	0.61346500	-0.10539000	-0.25172100
O	1.50765700	-0.53703700	-0.21129200
H	1.23555100	-1.45156500	-0.07568900
H	4.19577500	0.58735800	-0.35923600
O	4.09794600	0.38202300	-1.29868400
H	3.20353100	0.01555700	-1.31794500
H	-3.52823000	1.08258900	-0.04467300
O	-3.51340500	2.04505300	-0.18432000
H	-2.56901500	2.17117000	-0.31562500
H	2.88814900	1.46010400	1.74287100
O	3.28184200	0.60957500	1.53939500
H	2.58688100	0.13989400	1.02660700
N	-1.66987200	-0.78135300	0.02890400
O	-1.03186200	0.28635500	-0.18908100
O	-1.05901800	-1.85099300	0.12520000
O	-2.90028600	-0.73875700	0.14291700

W4\_S14

-1 1			
O	0.67654000	2.51730600	-0.67366000
H	-0.06884700	1.95184700	-0.42299100
H	1.41458500	1.89902400	-0.60379900
O	4.75951100	-0.69047200	0.48747000
H	5.06976200	-0.21472600	-0.28465500
H	3.79955100	-0.51081600	0.49201400
O	2.08906800	0.10972900	0.33069900
H	1.33391400	-0.40294900	-0.06318600
H	1.70255200	0.49606400	1.12076400

O	-4.10423400	0.35580300	0.79447100
H	-3.36845200	0.93513600	1.01341100
H	-3.63100300	-0.32545600	0.28827400
N	-1.09110000	-0.71522800	-0.29323700
O	-1.08433900	0.37269600	0.32135900
O	-2.15269700	-1.29602200	-0.53250400
O	-0.01064400	-1.22173100	-0.66373300

W4\_S15

-1 1			
H	-1.48201400	1.65463800	0.42674000
O	-2.23652300	1.26289500	0.91709900
H	-2.80314200	0.87471600	0.23593400
H	0.72834100	2.43871800	-0.04448400
O	-0.00731700	2.05332500	-0.52948200
H	0.35510500	1.14994500	-0.70604400
H	-4.14287100	-1.26824700	-0.16295900
O	-3.50661600	-0.87480300	-0.76328100
H	-2.63764100	-1.19411000	-0.42407300
H	-0.35254100	-1.28255300	0.17700500
O	-1.21838100	-1.39680300	0.61648100
H	-1.39688500	-0.52052400	1.00183800
N	2.19581000	-0.33222800	-0.06755500
O	2.64150200	0.79627100	0.17200300
O	2.80945400	-1.35066600	0.22666400
O	1.06300300	-0.43109200	-0.64336800

W4\_S16

-1 1			
H	-0.47472000	0.91032900	-0.55678900
O	-1.10109000	1.64823400	-0.71262200
H	-1.62472700	1.62586300	0.10106900
H	-1.37762900	-0.08840700	1.61407500
O	-2.30214900	0.18805400	1.57531500
H	-2.62640900	-0.32115900	0.81307200
H	-1.54216800	-1.33348500	-0.77655000
O	-2.43371400	-1.04453300	-1.03803100
H	-2.26291500	-0.14429300	-1.34793700
H	1.88473600	1.74398500	0.07658400
O	1.64858800	2.68272000	0.01109700
H	0.72799300	2.65848100	-0.27755100
N	1.33542200	-1.07013400	0.05344600
O	2.22689000	-0.21445800	0.06641500
O	0.11993300	-0.68784600	0.03784100
O	1.58502800	-2.26721700	0.05747500

W4\_S17

-1 1			
H	1.53934500	-1.45211700	-1.13785900
O	0.99987600	-2.19263600	-0.83633900
H	0.09558200	-1.82221400	-0.75445300
H	3.54423300	0.60404800	-0.20874500
O	2.63523400	0.40724700	-0.43966600
H	2.21647300	0.06539000	0.39382700
H	1.42977200	2.00737600	-0.58040800
O	0.75690300	2.69301600	-0.46394300



H	0.01346500	2.20267300	-0.08515900
H	0.43321400	-0.28526100	1.37656400
O	1.28775800	-0.73641200	1.57172400
H	1.22714700	-1.53260200	1.01634800
N	-1.81659700	-0.03612800	0.03634600
O	-1.54682700	-1.17457600	-0.39936800
O	-2.90447600	0.47703500	-0.18131200
O	-0.95134900	0.58452600	0.71458500

W4\_S18

-1 1			
H	1.07572800	1.50004000	2.02192800
O	1.19128800	1.13298000	1.14362500
H	0.47669500	0.45222200	1.06508300
H	0.81761900	-2.03953900	-0.02922800
O	1.04398300	-1.85285300	-0.94614900
H	0.36403500	-1.19058300	-1.17133100
H	-0.71440700	1.85582700	-1.17173400
O	-0.21384000	2.65323900	-0.95471700
H	0.41318400	2.32136100	-0.29627700
H	2.84212200	0.19789100	0.47870100
O	3.40772500	-0.45051400	0.03626300
H	2.76290900	-0.96381700	-0.47506200
N	-1.67809700	-0.45024000	0.17189000
O	-1.23713500	-0.15423800	-0.96415400
O	-0.85339100	-0.63125500	1.10977600
O	-2.87503100	-0.57007400	0.37219400

W4\_S19

-1 1			
H	-1.35064600	1.44693800	0.63380400
O	-2.01659000	0.87974700	1.08089000
H	-1.56316900	0.02176400	1.16911300
H	-1.78099200	-1.58328100	-0.20356900
O	-1.09898100	-1.74792700	0.46178300
H	-0.25887000	-1.49098200	0.03353000
H	-4.20973100	-0.85552400	-0.17915500
O	-3.53568200	-0.45846300	-0.73399500
H	-3.07173000	0.17220600	-0.13212200
H	0.78006000	1.79748700	-0.09669400
O	-0.07691000	2.14715700	-0.44607500
H	-0.21842800	1.53673400	-1.17686400
N	2.12251400	-0.25491700	-0.09030000
O	2.23161700	0.92832000	0.30661600
O	2.98408500	-1.08280400	0.17604100
O	1.11444900	-0.57364500	-0.77225300

W4\_S20

-1 1			
H	3.49068700	-0.40977300	0.29938000
O	4.16892100	-0.36627700	1.00580700
H	3.68916100	0.00571200	1.74775400
H	-0.59194200	-2.01794200	-1.63117700
O	-0.31806700	-1.96202600	-0.71312500
H	-0.60671700	-1.05386300	-0.42596400
H	1.51176600	0.34516600	-0.76771900
O	2.11329400	-0.41959500	-0.85766600

H	1.50844200	-1.17241400	-0.77415600
H	-2.82172400	-1.05582200	0.75575300
O	-2.98685400	-2.00763100	0.75385300
H	-2.15533400	-2.35163400	0.40435000
N	-0.89819200	1.49213200	-0.03506100
O	0.21568400	1.64925200	-0.56666400
O	-1.32797200	0.31747700	0.15562600
O	-1.58213000	2.44700500	0.30182000

W4\_S21

-1 1			
H	3.51962300	1.33696500	-0.18875700
O	3.72810300	2.19619100	0.22978100
H	2.87222600	2.52337800	0.51274100
H	1.98084100	-0.22542300	-1.03279700
O	2.93989600	-0.25601800	-0.86732400
H	2.98704900	-0.95117200	-0.19357500
H	1.13780200	-1.80812500	0.46283600
O	1.86277700	-2.20740800	0.99604300
H	1.73176100	-1.85034400	1.87665500
H	-0.46621600	-1.15107300	-1.17940900
O	0.18386000	-0.75499700	-0.58772800
H	-0.43058800	-0.14291300	-0.07084100
N	-2.69510500	0.33581800	0.04890700
O	-1.61550800	0.67594400	0.61929000
O	-2.65327800	-0.48962900	-0.87991600
O	-3.75419400	0.82566500	0.42370400

NO3(H2O)\_5]- Clusters

W5_S1			
-1 1			
O	-2.58453400	0.73793900	0.11162300
H	-1.97640000	1.00900000	0.83130600
H	-2.44839300	-0.21971600	0.06677800
O	-0.49781100	1.20362600	1.92386800
H	-0.20512300	0.28054700	1.89816500
H	0.11717000	1.66071400	1.30822200
O	-0.67641000	1.16541700	-1.92316200
H	-1.44647800	1.11344700	-1.32107700
H	-0.31825400	0.26504900	-1.90438600
O	1.15707500	2.24112800	-0.05892500
H	0.55725100	1.99520600	-0.79197300
H	1.85577700	1.56233400	-0.08882400
N	-0.09703500	-1.57863500	-0.00607800
O	-1.28986200	-1.87595800	-0.10724100
O	0.58129200	-1.36469900	-1.04203000
O	0.44415900	-1.47750800	1.10949200
O	2.83415200	-0.08711700	-0.04910100
H	2.13972300	-0.58986300	-0.52613100
H	2.65948200	-0.36889000	0.85427400

W5\_S2

H	-0.65010700	1.47633400	-0.77169900
O	-1.26436400	1.94266300	-0.17735300
H	-2.04884400	1.36439200	-0.14897100
H	0.42361000	-0.48456700	2.01318000

O	0.46195100	-1.45307800	1.86700800
H	1.16952200	-1.54558800	1.21131900
H	1.29006300	1.42644600	1.27588700
O	0.53247100	1.36653300	1.87600600
H	-0.20874900	1.64410000	1.29659100
H	-2.63337300	-0.72816700	-0.18323700
O	-3.32789900	-0.01826700	-0.22168200
H	-3.66903300	-0.06679600	-1.11666600
H	-0.83387100	-1.78193800	0.58684900
O	-1.32056200	-1.78502300	-0.26370700
H	-0.69164800	-1.33422700	-0.85878600
N	1.53399300	-0.01261900	-0.89999900
O	0.44298100	0.04857100	-1.52388000
O	2.00261200	-1.11984700	-0.60177400
O	2.11212000	1.03324000	-0.58017700

W5\_S3

O	-0.96920300	1.19353000	-1.72015100
H	-0.70355700	1.91590900	-1.11861300
H	-0.33446400	0.50506200	-1.46463300
O	0.17395900	2.65964800	0.41068500
H	-0.36277800	2.14656900	1.03971000
H	0.96514900	2.10322900	0.29824900
N	1.91938300	-0.45305100	-0.08585900
O	0.65933200	-0.64126400	-0.17667100
O	2.32599400	0.70392200	0.07930500
O	2.67806400	-1.40491100	-0.16234900
O	-1.25214600	-2.58901300	0.07194900
H	-0.42297000	-2.10340100	-0.11423200
H	-1.32465600	-2.54227600	1.02866500
O	-2.95015100	-0.22625900	-0.30788200
H	-2.40524900	0.32064000	-0.90938300
H	-2.52820100	-1.10081600	-0.33799900
O	-1.15898200	0.49327300	1.77021300
H	-0.44058500	0.08119500	1.26242100
H	-1.93331300	0.33384300	1.19603400

W5\_S4

-1 1

O	-0.98748600	1.75326200	1.42777400
H	-0.11211300	1.38695500	1.23347600
H	-1.55207800	0.96513000	1.55648800
O	-2.52340800	-0.63047400	1.41499400
H	-2.83662200	-0.52983200	0.49621700
H	-1.79300600	-1.25646900	1.28644900
O	-1.02043700	1.74992600	-1.38873400
H	-0.12922200	1.37629700	-1.32981000
H	-2.09257600	0.23530900	-1.54524800
O	-2.56417200	-0.61402500	-1.42635900
H	-1.19035600	1.96878600	-0.45144100
H	-1.85317800	-1.23970700	-1.21909000
N	2.32445500	-0.05955000	-0.01096600
O	2.60722100	-1.25964500	-0.00690500
O	1.08611300	0.27018000	-0.02420200
O	3.17287700	0.81905500	-0.00413500
O	-0.40979600	-1.92759800	0.01439900
H	0.17968400	-1.12459600	-0.00161300

H	0.22098700	-2.65047700	-0.00333300
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W5\_S5

-1 1

H	3.52807800	-0.33142700	-0.00612400
O	3.09755000	-1.18942000	-0.00438500
H	2.40525000	-1.10512900	-0.70736800
H	0.28932400	-0.95187800	-1.27259000
O	1.09542100	-0.70008100	-1.75931100
H	1.11868600	0.27531900	-1.67904700
H	0.89026800	1.99149300	-0.27891200
O	1.19624300	2.04352600	-1.22775000
H	0.48434500	2.49908100	-1.68164500
H	1.80975000	-1.02004700	1.40289600
O	1.06324100	-0.77557400	1.97878500
H	0.27407000	-0.97464600	1.44284300
H	0.69308900	1.00952800	1.64521100
O	0.25801000	1.79271500	1.25110600
H	-0.63892100	1.44670100	1.04633300
N	-2.09493900	-0.39368700	-0.06485600
O	-3.02198000	-0.81680200	-0.74000100
O	-2.17277500	0.71183200	0.50941500
O	-1.03938000	-1.07659500	0.05994000

W5\_S6

-1 1

H	3.52807800	-0.33142700	-0.00612400
O	3.09755000	-1.18942000	-0.00438500
H	2.40525000	-1.10512900	-0.70736800
H	0.28932400	-0.95187800	-1.27259000
O	1.09542100	-0.70008100	-1.75931100
H	1.11868600	0.27531900	-1.67904700
H	0.89026800	1.99149300	-0.27891200
O	1.19624300	2.04352600	-1.22775000
H	0.48434500	2.49908100	-1.68164500
H	1.80975000	-1.02004700	1.40289600
O	1.06324100	-0.77557400	1.97878500
H	0.27407000	-0.97464600	1.44284300
H	0.69308900	1.00952800	1.64521100
O	0.25801000	1.79271500	1.25110600
H	-0.63892100	1.44670100	1.04633300
N	-2.09493900	-0.39368700	-0.06485600
O	-3.02198000	-0.81680200	-0.74000100
O	-2.17277500	0.71183200	0.50941500
O	-1.03938000	-1.07659500	0.05994000

W5\_S7

-1 1

H	0.60304700	-1.69990600	0.48035800
O	0.83435200	-1.91781500	-0.44657300
H	0.82568100	-1.04836000	-0.88306900
H	2.70422800	0.41781300	0.05452800
O	3.39156000	-0.26431500	0.01500000
H	2.88251400	-1.07146700	-0.12331300
H	-1.46093600	-0.54207100	-1.65324500
O	-1.87204100	-1.38052800	-1.38658200
H	-1.09438500	-1.89772200	-1.11650700

H	-0.89153700	-0.65895200	1.84553100
O	0.04788600	-0.85996100	2.03795400
H	0.50363100	-0.02597900	1.86016200
H	-2.45886800	-0.68164700	0.25942000
O	-2.50050500	-0.15738300	1.08353400
H	-2.22814100	0.72528200	0.78916800
N	0.04314200	1.39855700	-0.38370500
O	1.01034400	1.46443200	0.39742300
O	-0.99972400	2.01702200	-0.14449800
O	0.12722500	0.68518600	-1.40964500

W5\_S8  
-1 1

O	-0.20257500	2.32269900	-1.11561100
H	-0.42340100	2.34487200	-0.16336600
H	0.65332900	1.86940500	-1.08705100
N	1.91718600	-0.67133500	-0.10247100
O	2.95952500	-1.30494000	-0.12501600
O	1.92724500	0.57997700	-0.04545500
O	0.80852200	-1.27396300	-0.13670400
O	-1.28977800	-0.72608500	1.81333000
H	-2.06790300	-0.79853300	1.23078200
H	-0.55115300	-1.01773500	1.25329000
O	-3.27680600	-0.96895700	-0.21273400
H	-2.59057100	-0.63073900	-0.84579200
H	-3.35833900	-1.90081700	-0.42467300
O	-0.13706500	1.83031700	1.64507200
H	-0.67936400	1.03578000	1.82128700
H	0.68669300	1.44831300	1.30380500
O	-1.23399900	-0.18574600	-1.75374200
H	-1.03910800	0.76786800	-1.64678500
H	-0.49103100	-0.60547500	-1.27732700

W5\_S9  
-1 1

H	0.63006500	1.94534500	-0.26517400
O	0.05712400	2.71256700	-0.49465200
H	0.19120200	3.32352200	0.23255400
H	0.15014700	-2.03012400	0.08502600
O	-0.79592600	-2.21351300	0.25485700
H	-0.99732900	-1.60700200	0.99702800
H	-0.17310000	0.10435600	1.64864100
O	-1.06307000	-0.06137700	2.00694300
H	-1.63532800	0.47814600	1.42426400
H	-1.64022400	1.88140600	-0.28960000
O	-2.42486500	1.37528900	-0.01066100
H	-2.47419500	0.61523300	-0.62062700
H	-3.29132700	-1.52108800	-1.29475300
O	-2.47678400	-1.05186800	-1.48403900
H	-1.79527300	-1.51245100	-0.92664800
N	2.09976100	-0.25476200	-0.11298300
O	1.90281000	-1.48094200	-0.10210800
O	1.27219000	0.50124600	0.47949300
O	3.07065000	0.23184600	-0.67481200

W5\_S10  
-1 1

O	1.21275900	1.45884300	1.16748000
H	1.62315900	0.62709300	1.47337500
H	0.30837400	1.17301800	0.91935000
O	2.63543300	1.78877200	-1.07581200
H	2.06667400	1.76108800	-0.26096400
H	3.50061800	2.05252000	-0.75753000
O	2.42322700	-1.02181300	-1.27615400
H	1.46777900	-1.15333500	-1.19409500
H	2.52902400	-0.05373200	-1.34761400
O	2.10298100	-1.20130400	1.53742800
H	2.49816300	-1.22638100	0.64570000
H	1.17672300	-1.39700400	1.32485800
N	-1.32079200	-0.64902300	-0.08272700
O	-2.35252200	-1.07221000	-0.60879800
O	-1.30162700	0.48476400	0.44252400
O	-0.29083400	-1.35556700	-0.06975100
O	-4.25492000	1.04424900	-0.13153700
H	-3.78822200	0.23427000	-0.39621100
H	-3.53271300	1.51976300	0.28918200

W5\_S11  
-1 1

H	-0.23882100	1.42593100	-0.58565900
O	0.70081300	1.33071200	-0.85563600
H	0.70691500	0.45548500	-1.30030300
H	2.38889500	1.48976400	-0.31651600
O	3.30091100	1.33375000	0.01079400
H	3.27370600	1.59865500	0.93270900
H	1.96683900	-1.23472600	0.98222400
O	2.63465500	-1.52501800	0.32992300
H	3.08206300	-0.69177800	0.11182300
H	-0.24752600	-0.52247000	1.41549500
O	0.61165400	-0.17226600	1.72436200
H	0.75865400	0.52257300	1.06507200
H	1.27930600	-1.58592500	-1.01527600
O	0.54618300	-1.33227400	-1.60781600
H	-0.25013500	-1.35842500	-1.05135100
N	-2.43574300	0.09464600	0.09302200
O	-1.66010800	-0.88923100	0.26799700
O	-3.64533900	-0.06913800	0.11970800
O	-1.94748200	1.22826400	-0.10050400

W5\_S12  
-1 1

H	-1.26958600	0.29201400	0.58685000
O	-1.25863800	0.87560000	-0.19930600
H	-0.31305000	1.15425000	-0.24131800
H	-0.83606100	-0.58424700	-1.39454800
O	-0.35084100	-1.39669800	-1.63096100
H	0.48996700	-1.24992100	-1.15616800
H	-1.03077100	-1.84418800	1.33883600
O	-0.68980500	-1.03905800	1.76634300
H	0.20655100	-0.93926100	1.40008300
H	-2.43353200	3.65152300	0.47239800
O	-2.99291900	3.05997400	-0.03370600
H	-2.43730400	2.26164100	-0.14088300
H	-2.60128400	-2.87338600	-0.14264900

O	-1.68052900	-3.09380100	0.01229000
H	-1.18503900	-2.57379800	-0.66828400
N	2.18074800	0.50603000	0.02064700
O	3.38375900	0.68306800	0.12261900
O	1.69452600	-0.65141200	0.17418700
O	1.41255600	1.45772200	-0.23632200

W5\_S13  
-1 1

O	3.10997200	-0.50105100	1.47285700
H	3.48896400	-0.47445900	0.57826100
H	2.25062400	-0.91015500	1.29880800
O	-2.85671700	1.84827600	-0.11569300
H	-2.04910600	1.30907000	-0.24895800
H	-2.74763800	2.20273200	0.76902400
O	-4.26600100	-0.65671200	0.25293300
H	-3.41456700	-1.10274500	0.16119000
H	-4.02274300	0.26576200	0.08130700
N	-0.36630900	-0.79766700	-0.16340200
O	0.76386200	-1.31876400	-0.13477700
O	-1.37741700	-1.48998300	-0.13749700
O	-0.45637400	0.45799300	-0.22144900
O	3.17117400	-0.08519500	-1.38277700
H	2.87318000	0.78741200	-1.06771500
H	2.36606400	-0.61399400	-1.28252000
O	1.95770200	1.90805300	0.24834800
H	2.35179700	1.33686100	0.92567600
H	1.09796500	1.48226200	0.07317800

W5\_S14

H	2.14553000	0.18678500	1.16311100
O	2.32622500	1.13168400	1.29427700
H	1.52304600	1.56651800	0.96394500
H	-2.17316600	2.40748300	0.00654100
O	-3.09320400	2.15970100	-0.14759500
H	-3.05433400	1.19152200	-0.14923700
H	3.40336900	-0.53111800	-0.87690800
O	3.92789900	0.27217500	-0.98454600
H	3.58470900	0.82118800	-0.26258300
H	0.93000600	-1.22489900	-0.17738300
O	1.81605500	-1.49508200	0.16846500
H	1.64071400	-2.33676900	0.59426100
H	-0.38386600	1.12542200	-0.23008600
O	-0.09802800	2.05427500	-0.05434200
H	0.22193500	2.36647200	-0.90411300
N	-1.52918500	-1.25632600	-0.06535200
O	-0.58997500	-0.53709700	-0.54397700
O	-1.27751700	-2.41262200	0.25645500
O	-2.65316000	-0.77032400	0.05250200

W5\_S15  
-1 1

N	0.21353000	-1.57596100	0.05971100
O	1.15161900	-1.83273300	-0.70474900
O	-0.87127300	-2.16090300	-0.05544400
O	0.35538700	-0.71464700	0.96338500

O	0.18287700	1.94850300	-0.07025900
H	0.00012000	1.10226800	0.36966100
H	0.80137600	1.68310100	-0.77506200
O	2.64506100	0.96086300	1.37902200
H	2.02526700	1.69113700	1.25468800
H	2.04914200	0.19123900	1.34753400
O	-2.74282900	2.23932900	-0.32825100
H	-2.89688600	1.34573600	0.01436500
H	-1.77784600	2.31239000	-0.35581000
O	2.34996800	0.66957400	-1.47663900
H	1.99419900	-0.23093700	-1.38065300
H	2.77670700	0.81121900	-0.61582000
O	-3.16126300	-0.60705900	0.28714400
H	-2.32884000	-1.10955900	0.39025600
H	-3.41432700	-0.78829200	-0.62079800

W5\_S16  
-1 1

O	-1.33122300	2.15339800	0.54657900
H	-1.36409000	2.03088400	1.49755600
H	-0.57931600	1.58866700	0.25827200
O	-2.97330200	0.10940900	-0.47507700
H	-2.61201800	0.96099800	-0.17125500
H	-2.19756400	-0.47081200	-0.41043400
O	4.21207500	-0.77314900	1.11827000
H	4.13793300	0.10153200	0.70853100
H	3.41673200	-1.20754300	0.78462200
O	3.40957500	1.34295800	-0.72218600
H	2.48071500	1.12484600	-0.49839400
H	3.63169200	0.66898100	-1.36937200
N	0.67248600	-0.70681100	-0.23500800
O	1.68369000	-1.38828100	-0.41406300
O	-0.43819700	-1.22864400	-0.11781500
O	0.78287900	0.55298800	-0.17228800
O	-5.49247600	-0.61647300	0.38038600
H	-4.56089100	-0.38130200	0.18637400
H	-5.88474900	-0.68621500	-0.49128700

W5\_S17  
-1 1

N	0.41046400	0.39350100	0.00214300
O	0.26175800	-0.82188500	-0.18580000
O	-0.57839000	1.14032700	0.10755400
O	1.55744200	0.88104700	0.08161400
O	2.21571700	-2.90450300	0.80553700
H	1.44269300	-2.35519800	0.62267100
H	2.93379700	-2.33888300	0.48577500
O	3.63682600	-0.83225200	-0.66741000
H	2.93683900	-0.22045800	-0.35919400
H	3.25200800	-1.23015000	-1.45171100
O	-5.40163000	-0.74874700	0.21475400
H	-5.73746700	-0.42265600	-0.62164400
H	-4.43248400	-0.69603700	0.10114700
O	0.96039700	3.74973500	0.29703100
H	0.06053500	3.40873100	0.29110900
H	1.45207100	2.91750200	0.24632000
O	-2.72082700	-0.54707100	-0.47825100



H	-2.09219200	0.16202900	-0.23776700
H	-2.13939200	-1.31260000	-0.49193800

W5\_S18

-1	1		
H	3.46914100	0.06072000	-0.04702900
O	3.30148600	0.45474100	-0.91581300
H	2.62827400	1.14840000	-0.76242500
H	-3.68682500	-0.80292900	-0.14347400
O	-3.91194300	-1.35768800	-0.90867900
H	-3.06512400	-1.35975200	-1.36434000
H	3.66459000	-2.20879400	1.08281400
O	3.13722000	-1.44942300	1.33822700
H	2.31421500	-1.54437100	0.80783400
H	0.50977300	1.84605100	0.04177800
O	1.08152600	2.12451000	-0.71099700
H	0.58805400	1.78679700	-1.46369200
H	1.84782500	-0.85213100	-1.02051100
O	1.23274600	-1.49333900	-0.62341300
H	0.39307800	-1.00716500	-0.51995700
N	-1.53364800	0.53840600	0.58509700
O	-0.73986400	1.30596500	1.15761500
O	-1.18546700	-0.03164400	-0.47921100
O	-2.65663500	0.34241900	1.05393800

W5\_S19

-1	1		
H	1.92089100	1.23280100	-1.53703100
O	2.27389500	1.03657800	-0.66622300
H	1.83231500	0.20365900	-0.38740500
H	0.99707000	-1.97431400	-0.38076400
O	1.29323300	-1.34464700	0.28611700
H	0.42114600	-1.10335500	0.69029200
H	-1.74040800	1.04785100	0.96695200
O	-2.04667200	1.95326000	0.75300900
H	-2.72987800	1.76542500	0.10310400
H	3.99220000	-0.11274400	-0.01045900
O	4.23014500	-0.93845300	0.42867100
H	3.36208000	-1.30853100	0.63520200
H	-0.53423900	2.85420000	0.01392600
O	0.27313900	3.24714800	-0.36160000
H	0.97046500	2.61046700	-0.16144900
N	-1.84033900	-1.19651200	-0.12717400
O	-1.22651500	-0.69084900	0.86844700
O	-2.92681100	-0.72888900	-0.45735500
O	-1.32157400	-2.13913300	-0.73133600

W5\_S20

-1	1		
O	-2.64535100	-1.53818800	1.74565400
H	-1.84396300	-1.05001200	1.52004800
H	-3.14436500	-1.48637000	0.91671900
O	3.84354900	-2.30103500	-0.93016300
H	3.89254100	-3.05326300	-0.33827600
H	3.24840900	-1.68199600	-0.45651700
O	2.53164400	2.10763800	0.60207300
H	1.56879000	2.08769100	0.40588600

H	2.93514900	2.28871800	-0.24943100
N	-0.85240900	1.10700000	-0.28177100
O	-0.08177100	2.07854100	-0.22239200
O	-0.50552200	-0.00629000	0.16878400
O	-1.97181200	1.24451500	-0.79245200
O	2.24108300	-0.70297900	0.64329300
H	2.55230500	0.21115800	0.76090300
H	1.29377200	-0.57815400	0.46208900
O	-3.30029900	-1.18462100	-1.07201200
H	-2.88062500	-0.30282100	-0.98096600
H	-2.54731500	-1.76461400	-1.21033600

W5\_S21  
-1 1

H	0.78219100	1.52089400	-1.15210600
O	0.15323200	2.16679300	-0.80585000
H	-0.68226700	1.66852300	-0.74628900
H	5.03005700	-1.45789600	0.07101000
O	4.85859300	-1.22581100	-0.84302600
H	3.98300600	-0.79249800	-0.80824000
H	-0.12327500	-1.87022100	1.37098900
O	0.22574500	-1.04468700	1.02988900
H	-0.55959700	-0.63382000	0.55817900
H	0.94352600	0.71973600	1.82132900
O	1.41435800	1.55359300	1.67099300
H	0.89147500	1.97900500	0.96513700
H	2.36861000	0.61971700	0.25404500
O	2.35131500	-0.02702900	-0.47561800
H	1.67574500	-0.65069900	-0.15123900
N	-2.80989600	-0.41086800	-0.22181100
O	-1.68462300	0.19146000	-0.23486800
O	-2.87984000	-1.49777500	0.35758500
O	-3.76880500	0.10512100	-0.77787200

W5\_S22  
-1 1

N	-0.91805400	-0.06654700	0.69010600
O	-1.13683200	-1.27762400	0.62226400
O	-0.05847500	0.38418500	1.46485400
O	-1.57506900	0.72744300	-0.03095400
O	-0.19350100	3.07123400	-0.46418100
H	-0.17306900	3.45772500	0.41431300
H	-0.72962500	2.25586900	-0.33697400
O	1.48054100	-2.77486500	0.20727800
H	1.92685600	-2.12607700	-0.35734600
H	0.66314500	-2.33893300	0.48243000
O	2.10708800	1.48130900	0.07736600
H	1.49347200	1.03946300	0.69163000
H	1.51278100	2.11675200	-0.35816400
O	-3.65182500	-1.00344000	-1.10574700
H	-3.07627700	-0.25567100	-0.88131300
H	-3.14641500	-1.72509300	-0.72011300
O	3.19184900	-0.74774000	-1.09016200
H	2.79256300	0.09839300	-0.78912600
H	3.85274300	-0.94062100	-0.42182000

W5\_S23

-1 1

H	0.30370900	2.72708000	-1.66281900
O	-0.02738400	1.83722100	-1.80026100
H	0.70114400	1.25966400	-1.47308200
H	1.35643300	1.17771700	1.20787400
O	0.81651500	1.31104100	2.01767600
H	0.94080200	0.47415100	2.47481800
H	-0.85749000	1.23398700	1.11445200
O	-1.56039900	1.08590200	0.45417000
H	-1.16859200	1.39169100	-0.38641700
H	-3.45781700	0.23480700	0.28546400
O	-4.06259200	-0.48370500	0.05738200
H	-3.44778300	-1.20544800	-0.12786900
H	-0.56959200	-1.91234400	-0.44255800
O	-1.39023700	-1.75097900	0.04018400
H	-1.36838300	-0.79560100	0.22490900
N	1.85266900	-0.68675300	-0.23536800
O	1.38018800	-1.37331500	-1.14362800
O	1.91705000	0.57636700	-0.38990400
O	2.25172000	-1.17483600	0.81848200

W5\_S24

-1 1

O	2.55216000	2.40630000	-0.13868500
H	2.61080700	1.45486300	0.03990100
H	1.62373300	2.53361000	-0.36731800
N	1.59310500	-1.25625500	0.13999800
O	1.67102500	-2.47535900	0.11851400
O	0.44555700	-0.70424600	0.04479700
O	2.58896000	-0.53513600	0.25224600
O	-1.80080700	-0.57966300	-1.58845300
H	-1.06877300	-1.03184200	-1.13100500
H	-1.48392800	0.34055700	-1.57748300
O	-3.73419800	-0.39979100	0.30946200
H	-4.30663700	0.30343600	-0.00288900
H	-3.09627700	-0.55037400	-0.42986300
O	-0.37538500	1.78776800	-0.71334600
H	0.17036500	0.99089500	-0.54751600
H	-0.87625100	1.83003300	0.11952600
O	-1.54141500	0.79846000	1.71759200
H	-2.34415400	0.35848200	1.38613200
H	-0.82779200	0.17746100	1.51352900

W5\_S25

-1 1

H	-3.16313100	-2.77929300	0.21698900
O	-3.26582500	-2.11671100	-0.46881100
H	-2.37358600	-1.71775900	-0.54583800
H	0.52867000	1.64585800	1.31802800
O	0.72661300	2.18482700	0.54744900
H	1.38511200	1.62306400	0.06681300
H	-3.68200600	-0.19358200	0.57390700
O	-3.15154200	0.46403700	1.04305400
H	-2.26077800	0.09454000	0.91455000
H	-0.00269700	-0.75025000	-0.01297800
O	-0.93884000	-0.66211400	-0.31011100
H	-0.99918300	0.17523900	-0.80669100

H	-0.78935600	2.22707500	-0.47722900
O	-1.57241700	1.99080400	-1.01647800
H	-2.27737000	1.81822600	-0.37675500
N	2.56830900	-0.55660400	0.02157700
O	2.53280400	0.52864900	-0.60296300
O	3.56525100	-1.26287500	-0.01066800
O	1.56097700	-0.90747800	0.69079800

W5\_S26

-1 1			
O	0.37807700	1.76999100	0.00057800
H	-0.31378500	1.16870900	-0.34535200
H	1.16504600	1.21125600	-0.07350500
O	3.94360100	-2.25929300	-0.59763300
H	3.08220300	-1.89553900	-0.31764100
H	4.34589100	-1.53192900	-1.07497100
O	1.59463100	-0.89253600	0.07136100
H	0.76905100	-0.97845400	-0.43718800
H	1.25822600	-0.79382900	0.98630800
N	-2.04249400	-0.96710000	-0.38793900
O	-2.95256200	-1.40130400	-1.07380800
O	-1.04402100	-0.41495400	-0.93959100
O	-2.07555500	-1.05631600	0.85601700
O	0.09619900	-0.13845400	2.28536900
H	0.14265000	0.75565200	1.92256300
H	-0.70050300	-0.50447700	1.83965000
O	0.55019300	4.51528400	-0.54732700
H	0.11406600	4.81569300	0.25161100
H	0.51010700	3.54327200	-0.47562200

[NO3(H2O)\_6]- Geometries Clusters

W6\_S1

-1 1			
N	-0.02602000	-1.45580300	-0.57150300
O	1.20191900	-1.56920000	-0.68234500
O	-0.60651500	-1.86104000	0.44945000
O	-0.68807100	-0.92970200	-1.49434200
O	2.51179200	-0.03863600	1.48190000
H	2.60807100	0.53988500	0.69692900
H	2.23371800	-0.86888000	1.07168800
O	-1.60105400	1.99766000	0.79057500
H	-2.25775000	1.34363500	0.49358500
H	-1.05324600	1.49707300	1.42912900
O	-0.11030400	0.24697300	2.38909600
H	-0.36025300	-0.55853600	1.91216700
H	0.84917500	0.30703300	2.20523700
O	2.49356100	1.05321600	-1.07756400
H	1.65881900	1.55545100	-1.19980500
H	2.22244500	0.15211900	-1.30236500
O	-3.07261100	-0.28290800	-0.17624700
H	-2.89756600	-0.89925700	0.54134700
H	-2.34275200	-0.50775400	-0.78724000
O	-0.07601400	1.94564700	-1.50882000
H	-0.58832800	2.09497100	-0.68279900
H	-0.31181200	1.03880500	-1.75096600

W6\_S2

-1 1

O	3.00691400	1.01512700	0.14347000
H	3.03928700	0.37202200	0.85817200
H	2.53810500	0.49792200	-0.54446700
O	-2.25774400	-1.20445700	0.96260700
H	-1.63898200	-0.73351300	1.56319400
H	-1.65192600	-1.67259900	0.36366700
O	-0.68497300	1.53574800	-1.64672900
H	-0.13878200	0.75054500	-1.80613900
H	-1.57280600	1.20315100	-1.41211700
O	0.49004300	2.25510000	0.79032800
H	1.41721300	2.01572800	0.61220800
H	0.04322500	2.10586800	-0.06984100
O	-3.19701900	0.78454400	-0.60343200
H	-2.91911300	0.02063000	-0.03641600
H	-3.31097400	1.50950400	0.01489000
N	0.85022700	-1.35757600	-0.60944300
O	1.42084200	-1.53652900	0.48125300
O	1.34445500	-0.55954600	-1.44161300
O	-0.19908900	-1.94811800	-0.88294500
O	-0.19527300	0.04806800	2.31754200
H	0.42433600	-0.57749900	1.91214700
H	-0.00641900	0.89177300	1.84696000

W6\_S3

-1 1

N	-1.71328700	-0.55876800	-0.53051000
O	-0.84114200	-0.56945700	-1.43813700
O	-1.71987600	-1.46933900	0.31628900
O	-2.53849800	0.35461400	-0.48764700
O	-0.96507600	2.34507100	0.98571300
H	-1.74493400	1.90875200	0.61526400
H	-0.36247800	2.38280000	0.21064000
O	0.88454800	-2.56533200	-0.63000100
H	0.33780400	-1.85898500	-1.04029900
H	0.23616200	-2.96318100	-0.04067600
O	3.03129100	0.97311400	-0.65799800
H	2.77834500	0.34005600	0.06555300
H	3.32004700	0.40816200	-1.37739600
O	2.23441400	-0.83810000	1.14803900
H	1.84459100	-1.51282100	0.55813800
H	1.46368400	-0.48461600	1.64278500
O	-0.12683100	0.04741600	2.33202400
H	-0.75463200	-0.54951800	1.90004500
H	-0.35996400	0.92731400	1.96450600
O	0.51614700	2.02081400	-1.33264800
H	0.01807200	1.21721700	-1.55337500
H	1.41648900	1.70578100	-1.11670100

W6\_S4

-1 1

O	1.25492100	-2.29685000	0.29834400
H	0.39302800	-2.25927100	-0.14320300
H	1.81235400	-1.71240500	-0.25922100
O	0.81232200	-0.38082100	2.31557600
H	-0.15715100	-0.30214600	2.30887100

H	0.99668800	-1.12776500	1.70924300
O	2.42616500	-0.32505200	-1.28112100
H	2.38890600	0.39925500	-0.61629300
H	1.60574700	-0.21826200	-1.78208800
O	-0.37556100	2.90769200	-0.15366600
H	-0.81618800	3.07351800	0.68284600
H	-0.85111100	2.13106200	-0.51559500
O	-2.06843700	-0.38301800	1.95927900
H	-2.08281900	0.01421100	1.06253600
H	-2.12076000	-1.32104100	1.75578000
O	2.02338000	1.55970700	0.70398300
H	1.61591700	0.95165300	1.35655200
H	1.28376500	2.10015000	0.37655700
N	-1.17314200	-0.34422800	-1.19277100
O	-0.41061500	-0.07468200	-2.11966900
O	-1.80430000	0.58661100	-0.61769900
O	-1.33992200	-1.50850600	-0.80335100

W6\_S5

-1 1			
H	0.26103400	0.33605000	1.84596600
O	-0.59120900	0.73666900	2.08831600
H	-1.24398700	0.03779500	1.88715400
H	-0.74121500	1.09288400	-1.38160700
O	-1.23134600	0.40251800	-1.88533300
H	-0.83754000	-0.43544700	-1.59012200
H	-3.61724100	1.24889500	-0.19138500
O	-3.62450400	0.41062200	-0.65907000
H	-2.79088800	0.42886800	-1.19767800
H	0.55861000	-1.54640800	-0.07275300
O	-0.17451100	-1.97117500	-0.59621100
H	0.24330800	-2.68442600	-1.08163200
H	-0.34034600	1.83654500	0.62875200
O	-0.00248000	2.20928700	-0.21170100
H	0.94676100	1.99990200	-0.17192400
H	-2.91280900	-0.80129900	0.57968400
O	-2.35295400	-1.31883300	1.18967000
H	-1.70244300	-1.74567200	0.61054600
N	2.46756100	-0.10925400	0.01035500
O	3.09526600	-0.87041800	-0.71530100
O	2.66716000	1.11127200	0.01203700
O	1.57755700	-0.58530600	0.78540700

W6\_S6

-1 1			
H	0.17276700	-2.22349500	-0.52551100
O	0.01211900	-2.46203300	0.40656200
H	-0.79598000	-1.95539300	0.61379000
H	3.66512700	0.07308900	-1.12243000
O	2.72631300	0.13372400	-0.94215000
H	2.57229500	-0.32214300	-0.05608000
H	0.95266800	1.88315700	1.33584500
O	0.60697500	1.23737800	1.97725600
H	-0.13585500	0.86709600	1.47137100
H	1.40675800	-1.59931200	1.10208400
O	2.13855800	-0.98245000	1.34062500
H	1.67384800	-0.21655500	1.74079400

H	1.29120800	-0.73436700	-1.88220800
O	0.41089900	-1.10293400	-2.06033700
H	-0.18480100	-0.47285000	-1.61808800
H	0.26116100	2.14962300	-0.68720300
O	1.14867200	2.50185600	-0.52575100
H	1.74337000	1.77534300	-0.77934200
N	-2.24777100	0.20008800	-0.03937300
O	-1.06859100	0.61004500	-0.29317800
O	-2.37363300	-0.84991200	0.61184600
O	-3.21233400	0.83622400	-0.42954800

W6\_S7  
-1 1

O	-2.33664600	1.26873000	-1.48461900
H	-2.09864900	0.35369800	-1.72182600
H	-2.98521100	1.11695800	-0.78251500
O	-0.27453400	2.12286500	0.29345000
H	0.57184700	1.73068300	0.01494400
H	-0.89545800	1.93290400	-0.43537500
N	2.95384000	0.00671800	-0.13128200
O	3.19051100	-1.16256900	0.19037100
O	3.82003700	0.86818700	-0.16192100
O	1.75544700	0.31580500	-0.44695300
O	0.19330700	-1.64907500	0.25284700
H	0.80001300	-0.91499400	-0.07347700
H	0.82193100	-2.33696500	0.48590200
O	-3.55123000	-0.16449400	0.72701400
H	-4.25309600	-0.25374500	1.37234000
H	-2.70206900	-0.04897000	1.24809300
O	-1.23150000	0.13025200	1.91351300
H	-0.70206300	-0.59538800	1.53209800
H	-0.86416000	0.92920000	1.46466200
O	-2.11002300	-1.58476800	-1.36338300
H	-2.74240800	-1.38309600	-0.65812400

W6\_S8  
-1 1

O	3.71433400	1.35860800	-0.20986100
H	3.55586000	0.40277900	-0.23203000
H	2.82015100	1.71900300	-0.12505300
O	0.77775200	1.71273900	-0.06711100
H	0.47631500	1.38547600	0.80672900
H	0.73031100	0.91805900	-0.62383100
N	-0.68584100	-1.35131500	-0.59310700
O	-1.87567500	-1.66680300	-0.53269100
O	-0.27690900	-0.58415200	-1.48634600
O	0.12336700	-1.78864600	0.25831400
O	-2.92587600	0.57862900	1.03437600
H	-2.69553100	1.16172600	0.28270100
H	-2.86807200	-0.30318900	0.63909100
O	-0.35652100	0.42478400	2.15435600
H	-1.30112200	0.54348900	1.92182900
H	-0.15316500	-0.45751800	1.81182300
O	2.90862400	-1.43564000	0.18556800
H	1.94927200	-1.54465700	0.03349900
H	2.98048800	-1.35221800	1.13897100
O	-1.84856800	1.87768300	-1.21671300

H	-0.99224200	2.14049600	-0.83460700
H	-1.62560100	1.02814800	-1.62650400

W6\_S9

-1 1

H	0.28745400	1.78341000	0.53009100
O	0.90779600	1.86607200	-0.22104700
H	0.91057000	0.98826600	-0.63212100
H	-1.79842300	1.85904800	0.56276700
O	-1.38015000	1.71139800	1.42825700
H	-1.69524000	0.83384100	1.70849800
H	2.27880800	-1.89589100	0.86019700
O	2.78302900	-1.56198100	0.11329000
H	2.07472800	-1.36506200	-0.52697400
H	-0.87226300	2.16861100	-1.32897500
O	-1.80798800	1.93019300	-1.40975900
H	-1.78533100	0.96766700	-1.54183800
H	2.84360200	1.60866300	0.46294300
O	3.67679300	1.17948000	0.70233700
H	3.49979000	0.23992500	0.54060000
H	-2.99525900	-0.89774400	1.06802000
O	-2.40637700	-0.96280900	1.82606300
H	-1.65288900	-1.44783700	1.43684800
N	-0.49732600	-1.23360100	-0.73119600
O	-1.64641400	-0.93454900	-1.08481600
O	-0.31300100	-1.95916200	0.26137300
O	0.48452800	-0.79460300	-1.36840700

W6\_S10

-1 1

O	-0.63205400	-0.56599800	-1.55611800
H	-0.95804800	0.35170800	-1.40438600
H	0.26823600	-0.59744800	-1.16795500
O	-4.11294300	0.17955100	-0.09154900
H	-4.31280600	0.11633200	-1.02811500
H	-3.51353700	-0.57631800	0.07694600
N	2.71971100	-0.11016200	-0.27835900
O	2.51550500	1.09723800	-0.06319400
O	3.83125500	-0.52491600	-0.56716900
O	1.74759200	-0.92363500	-0.19637700
O	-0.05125900	-0.91597300	2.01496300
H	-0.83035300	-1.25851900	1.55154100
H	0.66318900	-0.99491700	1.35607500
O	-2.15260900	-1.75559500	0.14719900
H	-2.21393700	-2.69446600	-0.03543600
H	-1.54123900	-1.36218600	-0.56145000
O	-1.74234200	1.81707200	-0.76694100
H	-1.10867400	1.92905700	-0.01756300
H	-2.55684800	1.47317600	-0.37095000
O	0.11680200	1.81435500	1.21933800
H	-0.05046400	0.97106700	1.67888800
H	0.95692800	1.63685600	0.74970400

W6\_S11

-1 1

O	0.53294100	3.16795500	-1.11816100
H	0.95685200	3.94722500	-0.75437500



H	-0.03973900	2.83268800	-0.38203900
O	0.90886400	-0.03038300	1.65405000
H	1.61223800	-0.70298200	1.64613500
H	0.14050400	-0.46205100	1.21678100
O	1.27668700	-1.79774200	-1.37595000
H	1.49593300	-0.84922600	-1.44363700
H	0.36546500	-1.79614200	-1.03450400
O	-0.78987100	2.19480400	1.01986700
H	-1.46927800	1.51959400	0.79197500
H	-0.11265900	1.67690800	1.47752700
N	-2.21692600	-0.83902200	-0.08361600
O	-2.61661300	0.24435100	0.38594200
O	-1.02667100	-1.20099600	0.14242900
O	-2.95374800	-1.55095200	-0.74673300
O	2.10540300	0.83810100	-0.79937800
H	1.65945600	1.65154600	-1.09859100
H	1.70245200	0.66720200	0.07249100
O	2.97670300	-1.80569000	0.78969200
H	3.52038300	-1.08953900	0.44824600
H	2.37730800	-1.99765300	0.03123700

# W6\_S12

-1 1

H	-2.63174100	1.40811700	-0.58594900
O	-3.60387400	1.32396900	-0.53382400
H	-3.81038200	1.54053900	0.37792400
H	0.56782400	-0.94587600	1.86186300
O	1.39412100	-0.59212100	2.23783200
H	2.05543600	-0.80496300	1.55879600
H	-0.17080000	1.11003100	-1.10290600
O	-0.82409900	1.33344200	-0.41477000
H	-0.24938000	1.73691800	0.27562500
H	1.30828500	1.20130400	1.75528900
O	1.24477900	2.02911000	1.23463700
H	1.78858300	1.83594900	0.45519500
H	-0.95660700	-0.38689900	0.27998300
O	-0.83831500	-1.31557400	0.56304400
H	-0.24545300	-1.65859400	-0.12624800
H	-3.81240100	-0.67429800	-0.20853500
O	-3.78511900	-1.54342800	0.21707300
H	-2.84173300	-1.68664800	0.37908800
N	1.94899500	-0.41289500	-1.01329100
O	2.87833200	-0.64657900	-0.22541200
O	1.21650800	-1.32685700	-1.42121500
O	1.73709400	0.76487400	-1.38575100

# W6\_S13

-1 1

N	1.91350000	-0.36347300	-0.16769700
O	2.63618400	-1.32504500	0.06732200
O	0.66508000	-0.52330800	-0.26221000
O	2.37439400	0.78168400	-0.32240700
O	-0.55770900	1.84711400	-0.26586200
H	-0.09035000	0.97384200	-0.33567100
H	0.16183800	2.47828000	-0.33594300
O	-1.60854600	-1.74855200	0.92853900
H	-0.71585300	-1.58049600	0.58471000

H	-2.18210800	-1.75796100	0.14079600
O	-2.29271900	0.79901800	1.85442500
H	-2.05826800	-0.13703100	1.67272300
H	-1.55637300	1.29230700	1.46252700
O	-3.46023300	-1.37743300	-1.21495800
H	-4.33721200	-1.60960600	-0.90395100
H	-3.41865500	-0.39421400	-1.13213600
O	5.20758900	0.31027100	-0.02426300
H	4.95492100	-0.60568600	0.12572700
H	4.32897600	0.70156300	-0.15896500
O	-3.31846100	1.28681800	-0.67646600
H	-2.43722400	1.62175200	-0.90866400
H	-3.20883600	1.15703000	0.28976900

W6\_S14

-1 1			
O	1.48982700	2.11234400	-0.92649200
H	0.55094300	2.33095900	-0.76841300
H	1.47995500	1.24789000	-1.35833000
O	-2.88867300	0.51070800	-0.55305900
H	-2.31470100	-0.04973300	-1.10155000
H	-3.00542800	-0.03324600	0.24566900
O	-1.03382900	2.44447600	0.24649800
H	-1.73458800	1.82143700	-0.03922000
H	-0.57513200	2.00150400	0.97384200
O	3.45505300	-0.99975700	0.76499400
H	3.02411600	-0.36555800	1.34943000
H	2.80436400	-1.10909200	0.05711300
N	0.11161700	-1.11990400	-0.89061900
O	-0.05597200	-1.31484500	0.34189100
O	-0.84822400	-1.18305400	-1.66154900
O	1.24962800	-0.85921600	-1.30667000
O	1.19000100	0.91420200	1.63799100
H	1.50637400	1.38133600	0.84071900
H	0.83528600	0.07888300	1.28726400
O	-2.49383300	-1.27684200	1.61202900
H	-1.66854000	-1.43626800	1.10507600
H	-2.19579000	-0.81290900	2.39767700

W6\_S15

-1 1			
O	0.07008900	-1.04459200	-1.34631500
H	0.97334600	-0.68791700	-1.50549100
H	-0.50022700	-0.25817000	-1.34725400
N	-1.58710400	0.91136800	0.53365700
O	-1.53784500	1.24119300	-0.67023400
O	-0.67012400	1.28138500	1.30962800
O	-2.50597000	0.21417800	0.95755900
O	0.67358200	-1.30504900	1.40334100
H	0.23227900	-0.50344600	1.72382200
H	0.37577700	-1.36000400	0.47212900
O	2.54511500	0.18585700	-1.40859800
H	2.8549300	1.03748300	-1.08879300
H	2.95965000	-0.21852500	-0.62460500
O	3.32626600	-1.12653500	0.99144000
H	2.37072400	-1.16809200	1.24750600
H	3.57260400	-2.04019900	0.83579400

O	-2.72720300	-2.17478100	-0.89415300
H	-2.83358600	-1.39291000	-0.33423900
H	-1.80473300	-2.13096700	-1.16932900
O	1.13947200	2.44922600	-0.48131400
H	0.64864000	2.09438500	0.28838600
H	0.42269900	2.48174300	-1.12434900

W6\_S16  
-1 1

H	2.34209000	-0.98830100	1.55828500
O	2.09380800	-1.92070100	1.54353200
H	2.40788000	-2.19487900	0.66268800
H	-2.00778600	-0.85540300	0.54558500
O	-2.76211300	-0.29075800	0.78611600
H	-2.46486900	0.61315300	0.57607000
H	0.01389900	-0.67774700	-0.41619100
O	-0.29768700	-1.53693900	-0.07316000
H	0.31387300	-1.73125500	0.65794400
H	-0.84085900	1.87506300	-0.43531200
O	-1.63595500	2.21984100	0.02215200
H	-1.25507900	2.74184600	0.73258500
H	1.51785700	-2.09918500	-1.33608200
O	2.47275600	-1.97178900	-1.26979800
H	2.55463500	-1.01841700	-1.08133700
H	-4.96554300	-0.78617400	-1.28910600
O	-5.19184200	-0.94943400	-0.37211600
H	-4.36139500	-0.73929700	0.10484000
N	1.59766600	1.35020600	-0.16392700
O	1.52595100	2.42397600	0.41748300
O	0.64969200	0.96845300	-0.90820700
O	2.59059500	0.60849400	-0.03756100

W6\_S17  
-1 1

O	2.25805900	-0.43766000	0.39568400
H	1.66781500	-0.78832500	-0.29522100
H	2.26408000	0.51403200	0.15550100
O	1.70153500	2.00827300	-0.78939100
H	1.32723100	1.40094700	-1.44274100
H	0.91668400	2.25199000	-0.24694300
O	0.39292300	-0.46824600	-1.69784300
H	0.22666500	-1.04402000	-2.44554300
H	-0.50554500	-0.26600500	-1.31641300
O	-0.01745700	-0.05206600	2.16499400
H	-0.70209500	-0.55531200	1.68575200
H	0.81684200	-0.29414200	1.73019000
O	-0.59468600	2.24961800	0.71872100
H	-1.22830900	1.79136100	0.14493000
H	-0.37903600	1.55590500	1.37898000
N	-2.68584000	-0.60865600	-0.16830800
O	-3.88825800	-0.71224200	-0.34202700
O	-2.08437600	-1.30203900	0.66887200
O	-2.02191900	0.22550000	-0.86514300
O	4.90546100	-1.33680000	0.01139200
H	3.97974100	-1.10740100	0.22102700
H	5.20654500	-0.59314100	-0.51342700

## W6\_S18

-1 1

H	-2.09175000	1.18344600	1.12818700
O	-2.25712400	1.84412300	0.42311800
H	-1.36387500	2.03250400	0.07748800
H	3.23277400	1.31438900	0.09590600
O	3.20435000	2.26958900	0.24993600
H	2.26494800	2.45677600	0.12453500
H	0.57865800	0.95673800	-0.35330400
O	0.38861700	1.91599000	-0.54327200
H	0.48656500	1.99785700	-1.49444500
H	-0.64602800	-0.30095100	1.99232300
O	-1.60510100	-0.30694800	2.09197200
H	-1.86878900	-0.97221100	1.41716600
H	-4.26146200	0.13299200	-1.18937300
O	-3.33608800	0.21350800	-1.42753700
H	-2.96768000	0.87674600	-0.78853900
H	-2.38873200	-1.26703300	-0.70833600
O	-1.94080000	-1.90752500	-0.12615200
H	-0.99001000	-1.74030400	-0.24692100
N	1.77443100	-1.26918100	-0.17562300
O	2.78296000	-0.59137800	-0.39408600
O	0.65900700	-0.67178500	0.00960300
O	1.80347500	-2.48890900	-0.13674800

## W6\_S19

-1 1

H	-3.03748500	0.94570800	-0.56701600
O	-3.47040300	0.16277300	-0.16933100
H	-3.09698800	0.11338500	0.73227900
H	0.69195500	-1.39921400	0.29296300
O	-0.25542000	-1.49202600	0.54057700
H	-0.76102900	-1.75645400	-0.24928600
H	0.94297200	1.31910000	0.38352200
O	-0.04247800	1.30590300	0.48325400
H	-0.22651200	0.35010500	0.41468400
H	-1.57104000	1.93324300	-2.09121300
O	-1.87410400	2.21552100	-1.22557500
H	-1.12050000	1.99298800	-0.61934500
H	-1.39096200	-0.73730500	1.86710400
O	-1.97499200	-0.05582400	2.24782700
H	-1.43835200	0.74088500	2.14297600
H	-2.75423900	-1.15939100	-0.98566400
O	-2.24820200	-1.91114200	-1.38762500
H	-2.76491700	-2.69400600	-1.18929100
N	3.08733900	-0.04797200	-0.13114500
O	2.33295300	-1.04795100	-0.18649400
O	4.28031100	-0.16459500	-0.38125500
O	2.61679900	1.07318700	0.17690900

## W6\_S20

-1 1

O	-1.09627000	0.32823400	2.24481600
H	-0.84506700	1.08107000	1.67442100
H	-0.44665900	-0.33441200	1.97402300
N	1.91808300	-1.15835400	-0.00196700
O	2.82778800	-0.32791100	0.00266800

O	0.71007000	-0.74659600	0.10928300
O	2.12537500	-2.35769700	-0.10507600
O	-2.54697300	1.15736300	-1.36062600
H	-2.91562300	0.63351200	-0.60069700
H	-3.24656900	1.74668400	-1.64547200
O	2.62167800	2.64679300	-0.37499100
H	2.80326200	1.70389700	-0.25633800
H	1.66254100	2.68977600	-0.26456300
O	-0.17524900	1.84923800	0.06920300
H	-0.93710400	1.78497100	-0.53169400
H	0.28312100	0.98584800	-0.02740200
O	-3.22602500	-0.49142100	0.62837600
H	-2.73660500	-1.17766300	0.13133000
H	-2.59324800	-0.22364300	1.32740000
O	-1.51362900	-1.81660100	-1.13214600
H	-0.64611100	-1.65518400	-0.70397200
H	-1.62263100	-1.05760300	-1.71532000

W6\_S21

-1 1			
H	1.49850200	-2.04056900	0.56357300
O	2.22399000	-1.42718000	0.80161900
H	1.77794500	-0.67784600	1.22792900
H	-0.35024700	-3.50901100	0.85109900
O	0.00433200	-2.98766100	0.12857500
H	-0.63016400	-2.23769900	0.03772600
H	1.64411200	1.45152700	0.20137100
O	1.98678600	1.95372900	-0.55427300
H	2.44450700	1.27800800	-1.08046800
H	-1.27219200	2.33090100	0.02733100
O	-0.59423300	2.97522500	0.30078900
H	0.14543900	2.83258800	-0.30799300
H	0.17719700	1.66500000	1.55397200
O	0.47223600	0.74344100	1.66398700
H	-0.24665000	0.25403300	1.20536700
H	3.02659100	-0.82680900	-0.62813000
O	3.50115800	-0.35915900	-1.35640100
H	4.34642600	-0.12427700	-0.96852500
N	-2.38114900	-0.24224600	-0.35333600
O	-2.54906600	0.98402900	-0.38378700
O	-1.38352700	-0.70660400	0.28283600
O	-3.14835300	-1.01333600	-0.90958400

W6\_S22

-1 1			
H	-1.50991600	3.07993300	-0.75995300
O	-2.42066700	3.06339100	-1.08117300
H	-2.72581200	2.20990400	-0.74259700
H	0.68620500	1.55998800	-0.12854900
O	0.02803000	2.14170600	0.32404400
H	0.50926500	2.42128700	1.10717000
H	1.60103600	-2.58384400	-0.79211800
O	1.00842600	-2.09940900	-1.37423800
H	1.31572200	-1.16834700	-1.23025400
H	-0.62305700	-2.10408300	-0.97465200
O	-1.59934400	-2.03197200	-0.81196100
H	-2.01078000	-2.18110000	-1.66503000

H	-2.00529100	-0.28192700	-0.15168800
O	-2.28662000	0.49363100	0.36360200
H	-1.46638600	0.99163100	0.53356500
H	-3.11162600	-1.02238200	1.57242900
O	-3.25498800	-1.97480900	1.66017000
H	-2.70624000	-2.31914500	0.94445900
N	2.60515600	0.14689100	0.33016400
O	1.79750300	0.35184500	-0.63962200
O	2.78889200	1.04662000	1.14498100
O	3.16511700	-0.94477100	0.41120700

W6\_S23

-1 1

H	-2.63038000	-0.64466600	0.65918500
O	-3.01425000	0.24618500	0.55776800
H	-2.25189700	0.78500500	0.29089400
H	2.48410100	2.62954100	0.10618500
O	1.84215500	3.27283200	-0.23554500
H	1.00105700	2.79977200	-0.20030600
H	4.00001300	0.66298900	0.06297700
O	3.49396500	1.08484000	0.76246400
H	2.74634200	0.46373000	0.86500400
H	0.08318200	0.59252100	0.03976300
O	-0.48077400	1.31311400	-0.31892300
H	-0.50674100	1.14414800	-1.26440400
H	-0.89719200	-1.70581800	1.62678400
O	-1.44472800	-2.07135300	0.92582200
H	-0.81814200	-2.09138100	0.17418300
H	-5.86925700	1.17619800	0.21113500
O	-5.49316500	0.74522900	-0.55788800
H	-4.58992100	0.50978600	-0.26198700
N	1.56067100	-1.40012700	-0.38029200
O	1.27478200	-0.61207300	0.57736600
O	0.63581400	-1.99841400	-0.94988600
O	2.72671900	-1.54547800	-0.71710000

W6\_S24

-1 1

O	3.14513500	-1.45251100	0.60980300
H	2.54053300	-1.27629800	-0.13426000
H	2.56804200	-1.89753300	1.23555800
O	1.55042000	2.13814100	-0.71231100
H	0.63107900	2.33392500	-0.47936100
H	1.49377300	1.23684200	-1.06176700
O	-3.80269800	1.30310600	1.10249900
H	-2.99364700	1.66599600	0.71945100
H	-3.68505100	0.34353900	1.01695400
O	-1.36922900	2.01483500	-0.54315900
H	-1.23697700	1.07326300	-0.78856100
H	-1.73974400	2.42357500	-1.32839800
N	0.05847000	-1.17471000	-0.71091800
O	-1.04345500	-0.65536200	-1.03390000
O	0.08541800	-2.11561300	0.07373900
O	1.10500600	-0.71711700	-1.20704800
O	-3.10541100	-1.49526000	0.65340700
H	-2.61275900	-1.89484200	1.37379600
H	-2.41081800	-1.31053000	-0.00948700

O	3.51878100	1.39366000	1.36901600
H	3.48957000	0.44318900	1.18535100
H	2.87497000	1.77080900	0.75077100

W6\_S25  
-1 1

O	-4.08640900	-2.25726800	0.03452800
H	-4.55364400	-1.42632900	-0.06643300
H	-3.14874800	-1.98789200	0.05960500
O	-1.87274000	3.95814900	-0.61650500
H	-1.52642100	3.16137400	-0.17059900
H	-1.50456900	3.89757600	-1.49955200
N	2.41128300	-0.09526200	-0.02556100
O	2.56171300	0.09211200	1.18916600
O	1.57992200	0.61990500	-0.66243500
O	3.03855100	-0.96243200	-0.62742100
O	-1.49458100	-1.18101000	0.05474500
H	-0.88878000	-1.38193000	-0.68899400
H	-0.94883100	-1.19904300	0.86504700
O	0.34004400	-1.38720600	-2.03324700
H	0.80776700	-0.57313100	-1.74310800
H	1.02759300	-2.05336200	-1.94698500
O	0.02034800	-0.46743900	2.33642300
H	0.95908700	-0.37973600	2.09295800
H	-0.33340300	0.40246000	2.09848000
O	-0.79111100	1.58585000	0.43616600
H	0.12495800	1.42110000	0.13240200
H	-1.25988500	0.78046400	0.15472800

W6\_S26  
-1 1

H	-3.45234700	-1.44279700	0.45197800
O	-4.01282400	-0.74747100	0.82572300
H	-3.55819200	0.06650900	0.57160300
H	1.31440800	1.73569500	-0.18771800
O	2.28967400	1.54997100	-0.24277600
H	2.69902900	2.41017700	-0.34956900
H	2.83078500	0.36895200	1.27504500
O	3.04902600	-0.47451300	1.70260000
H	2.24412500	-0.99868900	1.55457600
H	0.34379500	-0.94129000	0.08293900
O	0.85077200	-1.74569200	0.29745900
H	1.55141100	-1.75265400	-0.37660600
H	3.56844000	-1.04392300	-0.19348200
O	3.27960200	-1.03425700	-1.12047200
H	2.92655900	-0.13419900	-1.19482200
H	-1.17665100	-2.55554500	-0.25662700
O	-1.99841400	-2.28135400	-0.68308400
H	-1.80632900	-1.35791500	-0.91217200
N	-1.14579900	1.40665000	-0.21166800
O	-0.26942600	2.25644000	0.04898100
O	-2.33078700	1.65656600	-0.02664100
O	-0.79067800	0.29520100	-0.67472500

W6\_S27  
-1 1

H	1.02621300	0.88342700	1.36601400
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O	0.37170300	1.44423100	1.83755000
H	0.52249100	2.30029000	1.41218000
H	0.10099000	2.41044400	-0.87917000
O	0.95398500	2.82849000	-0.68041900
H	1.57345600	2.08404300	-0.68300600
H	-1.47877100	-1.54295700	0.48187600
O	-1.62376700	-1.54074000	-0.48715800
H	-0.76555500	-1.83886900	-0.81766600
H	-0.50219700	-0.44124600	2.33391300
O	-0.53338700	-1.36998900	2.07382800
H	0.26489400	-1.48490000	1.51919400
H	-1.09866200	1.31374900	0.50700200
O	-1.51315200	1.29088700	-0.37211800
H	-1.47239800	0.34498100	-0.60706600
H	-3.57954000	-0.75849500	-0.88662800
O	-4.18386400	-0.00716400	-0.85130300
H	-3.58943800	0.72279600	-0.63626200
N	1.98090800	-0.81475600	-0.50672000
O	2.15251800	0.24798600	0.14432900
O	2.50185300	-0.96170500	-1.59958000
O	1.26563100	-1.71824200	-0.01054700

W6\_S28  
-1 1

O	5.00864700	-0.67473500	-1.08189600
H	4.32372800	-0.01687100	-1.25904600
H	4.73042900	-1.02351500	-0.22377500
O	0.46512800	2.69274800	-0.03289300
H	0.64119600	3.09192400	0.82137000
H	-0.21945900	2.01521400	0.15492200
O	0.85397300	-1.39421400	0.12288200
H	0.11921200	-0.79015600	0.39254600
H	0.41079200	-2.09021600	-0.36666800
O	3.42290000	-0.88624700	1.43911800
H	3.26195200	-0.04828600	0.97812900
H	2.61422300	-1.37322800	1.22579700
N	-2.16592100	0.12964400	0.23828900
O	-3.05651100	0.96723200	0.15672100
O	-1.00743200	0.48467000	0.61208800
O	-2.35342900	-1.06487200	-0.02973600
O	2.48063100	0.80854600	-0.69937800
H	1.90541700	0.02497600	-0.67945000
H	1.87304600	1.55786000	-0.55725500
O	-5.20220700	-1.03772900	-0.63566300
H	-4.28812100	-1.32458200	-0.48787500
H	-5.10456400	-0.09382900	-0.47666600

W6\_S29  
-1 1

H	-2.55491300	1.86866600	1.13634300
O	-1.61396500	1.80377600	1.33238600
H	-1.47312800	0.84733000	1.11828500
H	1.34651600	1.77560400	-0.80361200
O	2.00466000	1.09368800	-1.04209300
H	1.52821000	0.23304000	-0.98956800
H	-0.58219400	2.74240100	-1.35541100
O	-0.06743500	2.93136600	-0.56763100



H	-0.62438300	2.57881500	0.17181800
H	4.83130400	0.70196400	-0.11384900
O	4.08427800	0.52243900	0.45918700
H	3.28742800	0.83515900	-0.05754100
H	3.65024800	-1.19421000	0.72144600
O	0.88893300	-1.38039700	-0.67904300
H	-0.02474400	-1.30872500	-0.33254600
H	1.43982200	-1.69293100	0.05359300
O	3.31643400	-2.11724600	0.75391300
H	3.48330300	-2.46153500	-0.12631300
N	-2.70222900	-0.90309000	-0.05883300
O	-1.54317000	-0.72885200	0.44198700
O	-3.56909500	-0.04357700	0.14643900
O	-2.92462300	-1.90668900	-0.72149600

W6\_S30

-1 I			
O	-0.74865200	-1.00870300	0.73304000
H	0.11167400	-0.73608300	0.32751300
H	-0.51692400	-1.34430500	1.60115000
N	2.32495100	0.58401000	0.06724300
O	1.69708100	1.63190500	0.29818100
O	3.55553600	0.57332600	0.12378300
O	1.70375200	-0.46713300	-0.22043400
O	4.27884900	-2.17874000	-0.37065500
H	4.21894500	-1.22776700	-0.18096900
H	3.35593000	-2.38053700	-0.54657500
O	-4.69780500	-0.14946200	-0.51472000
H	-3.92928000	0.39852600	-0.22411600
H	-5.24734600	-0.20799300	0.26922900
O	-3.11922500	-2.59252200	-0.16162400
H	-2.25971100	-2.17840400	-0.00889700
H	-3.69413200	-1.85060100	-0.40763100
O	-2.56420500	1.12115800	0.53979100
H	-2.00347800	1.77513700	0.08084900
H	-1.95345600	0.37806100	0.70256600
O	-0.61385600	2.75602900	-0.61937300
H	0.17526300	2.21773800	-0.39369900
H	-0.46394300	3.58129300	-0.15403100

W6\_S31

-1 I			
H	-4.02985000	0.99211600	-0.22784400
O	-3.73922300	1.91642300	-0.27720200
H	-2.77413800	1.86611300	-0.24299200
H	0.55914600	-1.21881700	-0.29544200
O	-0.37134700	-1.19584100	-0.59325100
H	-0.56869800	-0.24406000	-0.66432500
H	-4.09444300	-1.11274500	-1.23356600
O	-4.36051100	-0.93555700	-0.32885700
H	-3.66204400	-1.36420900	0.21485600
H	-0.56225000	2.04654000	-1.33846100
O	-0.81323800	1.61333800	-0.52029500
H	-0.07400000	1.79653400	0.12055200
H	-1.51032900	-1.81030600	0.46835500
O	-2.27052800	-2.05980100	1.05817500
H	-2.10222900	-1.59093900	1.87816400

H	2.00895000	2.29293300	0.85389000
O	1.23348500	1.81792200	1.16898600
H	1.54695600	0.88024700	1.05092800
N	3.17540800	-0.38133200	-0.16458500
O	3.67608600	0.74861800	-0.11302600
O	2.10818600	-0.60370500	0.50149300
O	3.66647400	-1.28440700	-0.82502500

W6\_S32

-1 1			
O	-5.33852400	-0.19683400	-0.98959900
H	-5.04221500	-0.66612300	-0.19629100
H	-4.63711600	0.45460500	-1.11094800
O	5.61224800	-1.04901400	-1.16245700
H	5.05012500	-0.90685700	-0.37409700
H	5.19321400	-0.51040400	-1.83584400
O	3.85082600	-0.56287700	0.94940000
H	3.37818300	0.28117000	0.79080500
H	3.11609500	-1.18298400	0.92023300
O	-3.70551600	-0.95496000	1.36824600
H	-3.43551300	-0.06574600	1.09256400
H	-2.97738500	-1.48961200	1.02287600
O	-2.62326300	0.93072500	-0.54355500
H	-2.29001400	0.03381100	-0.71262100
H	-1.80045300	1.41603000	-0.37115800
N	1.05991800	1.06551000	0.21065400
O	2.17599100	1.57364000	0.38350600
O	0.93067600	-0.18054200	0.33951600
O	0.09145100	1.76894900	-0.08396100
O	-1.30167800	-1.53792800	-0.23504300
H	-1.01091400	-2.14637700	-0.91600800
H	-0.50111400	-1.00535700	0.00749300

W6\_S33

-1 1			
O	-4.64611200	1.24531500	0.68915800
H	-3.80551300	1.69945000	0.79457300
H	-4.34043400	0.39437600	0.33570000
N	-1.99563500	-0.64064100	-0.33014000
O	-3.16370600	-1.02484600	-0.33428100
O	-1.08596400	-1.37230100	-0.76804800
O	-1.70943800	0.49967100	0.11085900
O	3.52865200	-1.99164400	-0.37294600
H	4.08016800	-2.57462900	0.15178600
H	2.61255800	-2.15296500	-0.04677200
O	2.85488300	3.25376400	-0.20677600
H	3.15212800	2.52627600	0.35452100
H	2.02787900	2.90723600	-0.56401100
O	0.71317800	1.22426300	-0.80411400
H	0.78942500	0.62966400	-1.55513100
H	-0.17205400	0.99266700	-0.42159100
O	2.73513800	0.47580000	0.95500500
H	2.01356400	0.72555500	0.34250700
H	3.24480700	-0.19196100	0.46888500
O	1.10803400	-2.00023000	0.84373400
H	0.31881800	-1.79020400	0.30549700
H	1.37076000	-1.15931400	1.24428600

W6\_S34

-1 1

O	-5.13943500	-2.57559300	0.59873400
H	-5.03884400	-1.96883600	1.33409200
H	-4.41149900	-2.32694300	-0.00510500
N	-0.91373900	0.65694600	0.01509400
O	-0.45797200	-0.50284600	0.11292700
O	-2.06011700	0.83125400	-0.43154000
O	-0.22204300	1.62509900	0.36283400
O	-2.97451700	-1.75275100	-0.96746700
H	-2.78980900	-0.79839300	-0.85903800
H	-2.14676300	-2.13180700	-0.65680300
O	-1.95292800	3.90274500	-0.17219900
H	-2.61054400	3.27718400	-0.48837000
H	-1.23782100	3.29588300	0.07521200
O	4.08925300	-0.93624400	-0.51465100
H	3.75474100	-0.74667700	-1.39262100
H	3.37551700	-0.63938700	0.10001800
O	6.82032400	-0.58673900	-0.10757200
H	7.00392800	-1.41747800	0.33377200
H	5.85396100	-0.61155900	-0.24808300
O	2.08231700	-0.12491000	1.09223300
H	1.19636800	-0.39963000	0.76825300
H	1.96787300	0.82889400	1.14662100